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LABORATORY STUDIES AND MATHEMATICAL MODELING OF NO_x FORMATION IN COMBUSTION PROCESSES

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Laboratory studies were conducted to investigate the basic factors affecting nitrogen oxide formation in the combustion of fossil fuels. A jet-stirred combustor and a multiburner (so-named because of its ability to burn gas, oil or pulverized coal fuels) were used. The jet stirred combustor was used to study NO_x formation in combustion under kinetically limited conditions. The combustion conditions were selected to be pertinent to stationary sources such as furnaces and boilers with peak temperatures ranging from 2500-3500 F. Preliminary experiments were performed with the multiburner which indicated the influence of heat losses and residence time on NO_x emissions in the combustion of methane/air. The multiburner was used as a rudimentary flow reactor to study the formation of nitrogen oxides in air at high temperatures. The mathematical model has been extended to allow calculations of NO formation under fuel-rich conditions. Particle combustion capability has been incorporated into the model and mixing effects can be handled with the macro-mixing option. This latter feature allows consideration of such combustion modifications as staged or "off-stoichiometric" combustion. Test cases have been run for the above options which indicate the correct order of magnitude predictions and the correct directional effect of combustion modifications on NO_x emissions.

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By
William Bartok
Victor S. Engleman
Eduardo G. del Valle

Final Report
prepared under Contract CPA 70-90

for the
Office of Air Programs
U.S. ENVIRONMENTAL PROTECTION AGENCY

ESSO RESEARCH AND ENGINEERING COMPANY
Government Research Laboratory
Linden, New Jersey

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FOREWORD

This report summarizes the work performed on the basic laboratory studies and NO mathematical model development portions of a "Systems Study of Nitrogen Oxide Control Methods for Stationary Sources - Phase II". This work was sponsored by the Environmental Protection Agency under Contract No. CPA 70-90 at the Government Research laboratories of Esso Research and Engineering Company. Dr. William Bartok was the contractor's Project Director, and Dr. Victor S. Engleman acted as the Principal Investigator for the basic studies reported herein.

The results of a field test program on the application of combustion modification techniques to utility boiler operations for NO_x emission control, performed under the above contract, are summarized in a separate companion report (No. GRU.4GNOS.71).

The skillful assistance of Mr. Terry Scheurman in the laboratory portion of the program and the helpful advice of Dr. Robert Goldstein of Esso Mathematics and Systems Inc. in the mathematical modeling are gratefully acknowledged.

Mr. Stanley J. Bunas was the EPA Technical Project Officer during the initial part of this program and Messrs. G. Blair Martin and David W. Pershing were Technical Project Officers during the latter part.

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SUMMARY

This report summarizes the findings of the laboratory studies and mathematical modeling portions of Phase II of a "Systems study of Nitrogen Oxide Control Methods for Stationary Sources" (Contract CPA 70-90). Laboratory studies were conducted to investigate the basic factors affecting nitrogen oxide formation in the combustion of fossil fuels. A jet-stirred combustor and a multiburner (so-named becuase of its ability to burn gas, oil or pulverized coal fuels) were used in these studies. The first-generation model of NO formation and decomposition in combustion processes was extended.

The jet stirred combustor was used to study NO_x formation in combustion under kinetically limited conditions. The key findings of these studies with the jet-stirred combustor are as follows:

- At the very short residence times prevailing in the jet-stirred combustor (on the order of 2 msec), substantial quantities of NO_x are formed in gaseous premixed hydrocarbon (methane or propane) - air combustion, under stoichiometric and excess air firing conditions. (In fact, peak NO_x concentrations have been measured under slightly fuel rich conditions.) The NO_x concentrations measured exceed those based on the Zeldovich mechanism in many cases by more than an order of magnitude, indicating that coupling occurs between NO_x formation and combustion kinetics.

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- With carbon monoxide as the fuel, containing trace amounts of hydrogen, the NO_x emissions from the jet-stirred combustor are very similar to those obtained with methane fuel, at equivalent mixture ratios and slightly higher temperatures.

- With hydrogen as the fuel, the NO_x emissions are reduced to much lower levels at all mixture ratios compared with methane at the same temperatures. Good circumstantial evidence for the coupling between NO_x and combustion kinetics has been obtained in experiments in which methane or carbon monoxide was mixed with the hydrogen fuel. In the presence of samll amounts of these gases, the NO_x concentrations measured increased when compared to the results for hydrogen at the same mixture ratio.

- Under fuel rich conditions, the amount of NO_x drops off precipitously in the jet-stirred combustor. This finding provides support for the optimized design of the two-stage combustion technique for NO_x emission control from combustion sources.

- All of the "bond-type" additives (NO, NO_2, NH_3 and $(CN)_2$ and CH_3NH_2) result in nearly equivalent NO_x formation, operating the jet-stirred combustor with excess air. The conversion between additive input and NO_x output is constant as the additive level is increased up to 3000 ppm equivalent NO_x. (Slight falloff was noted for $(CN)_2$ above 3000 ppm.)

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- The fraction of N-bond additives oxidized to NO_x is sharply decreased on the fuel-rich side. This finding is of practical significance, because of the potential of fuel-rich combustion followed by second-stage air injection to control NO_x emissions resulting from both atmospheric N_2-fixation and fuel nitrogen oxidation.

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Preliminary experiments were performed with the multiburner which indicated the influence of heat losses and residence time on NO_x emissions in the combustion of methane/air. The multiburner was ~~has also~~ been used as a rudimentary flow reactor to study the formation of nitrogen oxides in air at high temperatures.

The mathematical model has been extended to allow calculations of NO formation under fuel-rich conditions. Particle combustion capability has been incorporated into the model and mixing effects can be handled with the macro-mixing option. This latter feature allows consideration of such combustion modifications as staged or "off-stoichiometric" combustion. Test cases have been run for the above options which indicate the correct order of magnitude predictions and the correct directional effect of combustion modifications on NO_x emissions.

1. INTRODUCTION

In Phase I of a "Systems Study of Nitrogen Oxide Control Methods for Stationary Sources" (1-1), sponsored by NAPCA (now the Office of Air Programs of the Environmental Protective Agency) under Contract No. PH-22-68-55, Esso Research and Engineering Company characterized the stationary NO_x emission problem in the U.S., assessed existing and potential control technology on the basis of cost-effectiveness, and developed a comprehensive set of five-year R&D plans for stationary NO_x emission control. In addition, a first-generation mathematical model of NO_x formation in gas-fired combustion processes was formulated, and knowledge gaps pertinent to the NO_x control problem were defined. This study identified the need for additional information on the mechanistic and kinetic details of NO formation in fossil fuel combustion processes.

The major portions of the stationary NO_x emission control problem studied during the present contractual period (Contract No. CPA-70-90) concerned high priority R&D needs identified in the Phase I study. These consisted of a systematic field investigation of modifying boiler combustion operations for NO_x emission control (the findings of the field study are reported in a separate companion report GRU.4GNOS.71), basic laboratory studies and extension of the kinetic model. The work performed on the laboratory studies and the kinetic model development is presented in this report.

Although studies of nitric oxides formation in combustion have been performed for over sixty years, major questions about the mechanisms and rates of formation still remain. Early experimental work in the field was conducted by Haber (1-2) and Bone (1-3) and tentative hypotheses included such concepts as quenching of equilibrium NO, participation of charged particles (ions and electrons), and nitrogen activation. However, it remained for Zeldovich (1-4) to postulate a thermal chain reaction involving nitrogen and oxygen atoms. Zeldovich found nitrogen oxide formation not to be dependent on the chemical nature of the fuel but only on its heat of combustion. He found that nitric oxide was formed after the fuel was completely burned. Even for fuel rich combustion of hydrogen, Zeldovich found good agreement with his chain mechanism.

This decoupling of the combustion reactions from nitric oxide formation has been used under selected conditions by Newhall (1-5), Lavoie, et al. (1-6) and Williams, et al. (1-7). These investigators have used additional reactions in the NO formation and decomposition, mechanism but combustion species are assumed to be in equilibrium before NO formation begins.

At the inception of this study little information was available about the NO_x emissions or mechanistic details under fuel rich conditions. While Zeldovich found his mechanism to give good predictions for fuel rich combustion of hydrogen (1-3), he did not report fuel rich results for hydrocarbon combustion. More recent work by Harris, et al. (1-8) has provided additional information on the effect of mixture ratios on NO formation in hydrocarbon combustion in flat flame burners.

Predictions of NO formation in hydrocarbon combustion under fuel rich conditions are particularly difficult. It is under these conditions that the interactions between combustion reactions and NO reactions are most likely to occur. In the absence of excess oxygen, decoupled kinetics can significantly underpredict NO concentrations. For example, the decoupled kinetic model used by Heywood (1-6, 1-9), which includes the Zeldovich mechanism as well as the N + OH = NO + H reaction, gave good agreement under fuel lean conditions, but underpredicted observed NO emissions under fuel rich conditions, in some cases by more than an order of magnitude.

The extent of these underpredictions of course depends on the interaction of a number of factors. Among these factors are (1) the validity of the simplifying assumptions made for the purposes of the model and (2) the accuracy of the available values for the key parameters of the model (including rate constants). The closest agreement with predictions has been obtained under fuel lean conditions in cases where post-flame NO formation is dominant (e.g., utility boilers emitting high levels of NO_x). The greatest difficulty has been found under fuel-rich conditions in cases where NO formation in the flame zone is important (e.g., a well-stirred combustor).

It has been established (1-1) that fuel nitrogen plays a role in NO_x formation. While quantitative data were not available at the beginning of this study on the rate of conversion of fuel nitrogen to NO_x, experimental work and emission correlations with fuel types indicated beyond a doubt the effect of fuel nitrogen on NO_x emissions. Flat flame experiments on the addition of nitrogen compounds to carbon monixide in low temperature combustion indicate conversions even under fuel rich conditions (1-10). Elshout and Van Duren (1-11) analyzed results of NO_x emissions from power plant boilers burning fuel oil of differing nitrogen contents. This analysis indicated a trend to higher NO_x concentrations with increasing nitrogen content of the fuels. Martin, et al. (1-12) studied the effect of nitrogen in fuel additives in an oil-fired furnace and generally found 30-40% conversion to NO_x. At low additive levels (ca. 0.05% N), however, they observed 60-70% conversions. The nitrogen compound type seemed to have little effect. Similar results were observed by Turner, et al. (1-13) who also studied the effect of flue gas recirculation on fuel nitrogen conversions in an oil-fired package boiler.

The possible participation of nitrogen-containing species such as CN and HCN as intermediates in NO formation was postulated by Fenimore (1-14). Subsequent studies (1-15, 1-16) appear to indicate that the rapid formation of NO in the flame zone observed by Fenimore possibly can be explained by high concentrations of oxygen atoms without resort to nitrogenous intermediates. Measurements have been made (1-17) which indicate that oxygen atoms can be present in substantial "superequilibrium" amounts (i.e., exceeding the equilibrium corresponding to the dissociation of molecular oxygen) in the combustion of hydrogen, carbon monoxide and hydrocarbons.

In order to obtain further information on the factors influencing NO_x formation in combustion at temperatures and pressures representative of conditions in stationary combustion equipment, an experimental study was initiated at Esso as part of the present EPA-funded program (Contract No. CPA 70-90). This laboratory study was designed to investigate NO_x formation under well-defined conditions. To this end, the jet-stirred combustor was used to study NO_x formation under conditions where combustion is not limited by mixing. In addition, a new laborabory device was designed, built and operated during this study. Called the "multiburner" because of its ability to burn gas, oil or pulverized coal, this device is capable of operating under conditions of controlled heat loss by maintaining the combustor walls at a specified temperature.

Predictive calculations of nitric oxide formation rates in a wide variety of combustion applications have been attempted. Three areas which have received attention in the published literature are the internal combustion engine, the gas turbine combustor and utility boilers. Much of the literature on the internal combustion engine was reviewed in reference (1-9) while a review on gas turbine modeling can be found in reference (1-18). Modeling and calculations related to utility boilers contemporary with our first generation model are reported in references (1-7) and (1-19). Williams, et al.(1-7) reported on a furnace model in which premixed fuel and air burned instantaneously on introduction to the furnace and cooled at a rate determined by radiative losses to the wall while in plug flow. More recently Williams, et al. (1-20) have reported on NO_x formation calculations in a diffusion flame which show promise for application to a utility boiler model. Calculations on NO_x formation in utility boilers were reported by Bagwell, et al. (1-19) in which a one-dimensional chemical kinetics program was used with a rather extensive set of chemical reactions. These calculations indicate peak NO_x formation at approximately five percent excess air with NO formation essentially proportional to the characteristic residence time at adiabatic combustion temperature.

The Esso first-generation mathematical model of NO formation in utility boilers (1-1) contained the following features:

1. One-dimensional, homogeneous gas phase reaction system.
2. Specified flow velocity, pressure, and flow area profiles.
3. Heat transfer specified optionally by
    a. heat transfer rate profiles
    b. heat transfer coefficients and wall temperature profiles
    c. gas temperature profiles
    d. quenching rate profiles.

4. Heat generation described by two-step overall kinetics of hydrocarbon oxidation to CO and H_2O, followed by CO combustion to CO_2.

5. Zeldovich-type kinetics used to calculate NO concentrations.

6. Multiple point injection of fuel, air or flue gases for simulation of two-stage combustion or flue gas recirculation.

The objectives of the second-generation development of the mathematical model were to:

1. Incorporate additional kinetics in the NO formation and decomposition reactions to allow use of the model under fuel-rich conditions.

2. Include analysis of particle combustion for use with oil and pulverized coal fuels.

3. Simulate the effect of mixing on a macroscopic scale.

This report summarizes the results of our laboratory studies and the development of our boiler-oriented mathematical model.

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2. LABORATORY COMBUSTION STUDIES OF NO_x FORMATION

Basic laboratory studies were carried out as part of this contract study, with the objectives of gaining a better understanding of the complex phenomena involved in NO_x formation in combustion processes, providing kinetic information relevant to the development of the NO_x formation model, and uncovering potential leads which may be useful to applied NO_x control technology.

Recent papers (2-1,2,3,4) have focused attention on the production of nitrogen oxides in both flame and post-flame zones. Since combustion conditions vary widely, it is conceivable that reactions that may be unimportant for NO_x formation in the internal combustion engine (2-1) might become important in gas turbine combustion (2-2,3); much of the recent controversy has centered on the nature of NO_x formation in the flame zone itself (2-3,4).

To sort out the phenomena affecting NO_x formation, idealized systems were used in the present study where the input conditions of fuel and oxidizer, the configuration of the combustor, the residence time - temperature history of the combustion gases were well defined. Also, because of the potential role of nitrogen compounds in the fuel and as intermediates in NO_x formation, known quantities of model compounds were added to the mixed gaseous fuel/air system. These studies provided useful information on the potential role and fate of nitrogen compounds under varying stoichiometric combustion conditions. Details of the experimental approach, the results obtained and their interpretation are discussed in this section of the report.

A number of techniques were used in the laboratory scale investigation of NO_x formation in combustion processes. A jet-stirred, premixed combustor has been used for NO_x formation studies under kinetically controlled combustion conditions, over a broad range of fuel/air mixture ratios. The effects of introducing nitrogen-bond type additives (NO, NO_2, NH_3, CH_3NH_2 and C_2N_2) have been investigated, to elucidate their potential role as intermediates in NO_x formation and provide information on the oxidation of nitrogenous compounds to NO_x. In addition to the jet-stirred combustor, a "multiburner" was designed and constructed during the course of the contractual period. Installation of this unit, which is capable of burning gas, oil or coal fuels at controlled rates of heat loss varying from adiabatic conditions to maximum cooling, has been completed and initial results on premixed gas flames have been obtained.

2.1 Apparatus

The jet-stirred combustor was the primary experimental tool used in the laboratory program during the contract period. This combustor, which closely approximates a perfectly stirred flow system, was developed by Longwell and Weiss (2-5) to study high temperature reaction rates in hydrocarbon combustion. Through the use of this device, we have been able to study NO_x formation in combustion under intensely back-mixed conditions which eliminated diffusional limitations. Thus, the reaction rates were limited by chemical kinetics and information was obtained on the kinetic limitations on NO_x formation in combustion.

The "multiburner" was designed to study the combustion of gas, oil, or pulverized coal under conditions of controlled heat loss. It is capable of operating at temperatures well in excess of 4000°F and at a wide range of combustion zone heat loss conditions including adiabatic operation.

Further description of the jet-stirred combustor and the multiburner is contained in the following sections.

2.1.1 The Jet-Stirred Combustor

The ideal perfectly-stirred flow system has a number of features that make it desirable for performing kinetic studies in combustion reactions. In such an ideal reactor, a homogeneous mixture of air and fuel enters the reactor and is mixed instantaneously with burning combustion gases in the reactor. The reactor contents, which are spatially uniform in temperature and composition, exit from the reaction zone at the same mass flow rate at which new reactants are being added. Ideally, the reactor is adiabatic and has minimum surface-to-volume ratio.

A practical stirred combustor approaches the ideal design and the jet-stirred combustor used in the current experimental program is a modification of the original Longwell reactor (2-5). The intense backmixing and turbulence in this combustor make it a very good approximation of the perfectly stirred flow system. It should be noted that because of this intense backmixing of the reactants with the products, the oxygen level is higher than it would be if the combustion reactions were allowed to proceed to completion. Thus, the oxygen concentrations are measurable even under fuel rich conditions. In fact, as the reactor approaches the rich blowout limit the measured oxygen concentration actually increases because the combustion is incomplete in the reaction zone. The high surface-to-volume ratio necessitated by the practical limits of gas flow rates results in some departure from adiabatic operation; however, since the temperature of combustion is measured continuously this departure from ideality results in a "well-stirred" system at a known, lower temperature.

The reactor (Figure 2-1) consists of an outer shell of fire brick shaped as two halves of a sphere three inches in diameter. The upper hemisphere is solid with the exception of the hole through which the reactants are brought to the injector. The lower hemisphere is hollowed out to a reaction zone of one and a half inch diameter. The insulating shell has twenty-five holes, 0.125 inch diameter, through which the burned mixture exists.

Fuel and air are metered separately through calibrated rotameters, preheated to the desired inlet temperature, and then mixed before entering the combustor. The fuel-air mixture enters the reaction zone through an Inconel injector which is a hemisphere into which are drilled forty radial holes 0.021 inches diameter. The reactants enter the reaction zone as small sonic jets which stir the reactor contents and produce a mixture of essentially uniform temperature and composition in a characteristic time which is short compared with the average residence time. The burned mixture exists through holes in the combustor shell, spaced as evenly as possible. A schematic of the control systems and the sampling train for the jet-stirred combustor is shown in Figure 2-2.

Gas temperatures were measured up to temperatures slightly in excess of 3200°F with a 0.010 in. diameter Pt/Pt-10% Rh thermocouple. The thermocouple was movable so that traverses could be taken during a run. It was found that the temperatures were quite uniform throughout the reaction zone, although somewhat cooler in the immediate vicinity of the injector sphere and in the immediate vicinity of the wall.

The combustion gases were sampled through a water-cooled stainless steel probe, 0.125 inches outside diameter and 0.033 inches inside diameter placed through a hole in the shell of the combustor. The probe was also movable and traverses were taken to assure uniformity of combustion zone composition. While some non-uniformities were noted on the extremely fuel-rich side, these occurred so close to blowout that they did not appear to affect the NO measurements. The quenched gases are pumped through a diaphragm pump to the combustion gas analyzers. An Envirometrics multigas analyzer was used to measure total NO_x and NO_2 (this instrument can also measure SO_2), a Beckman paramagnetic analyzer was used to measure oxygen, and a dual column gas chromatograph was used to separate N_2, O_2, CO, CO_2, H_2 and hydrocarbons. The water content of the gases was handled in one of two ways. It could be calculated from an oxygen balance by comparing input N/O ratio with output N/O ratio and attributing the difference in oxygen to water, or it could be calculated from a hydrogen balance by comparing the input C/H ratio with output C/H ratio and attributing the difference in hydrogen to water. These two methods provided a good cross-check on the mass balance and mixture ratio.

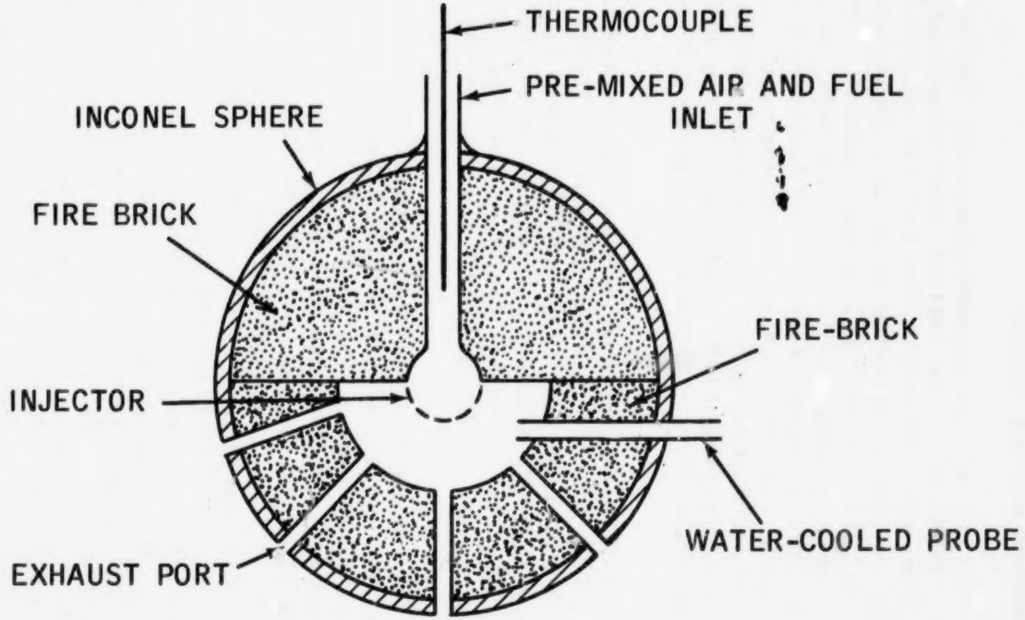
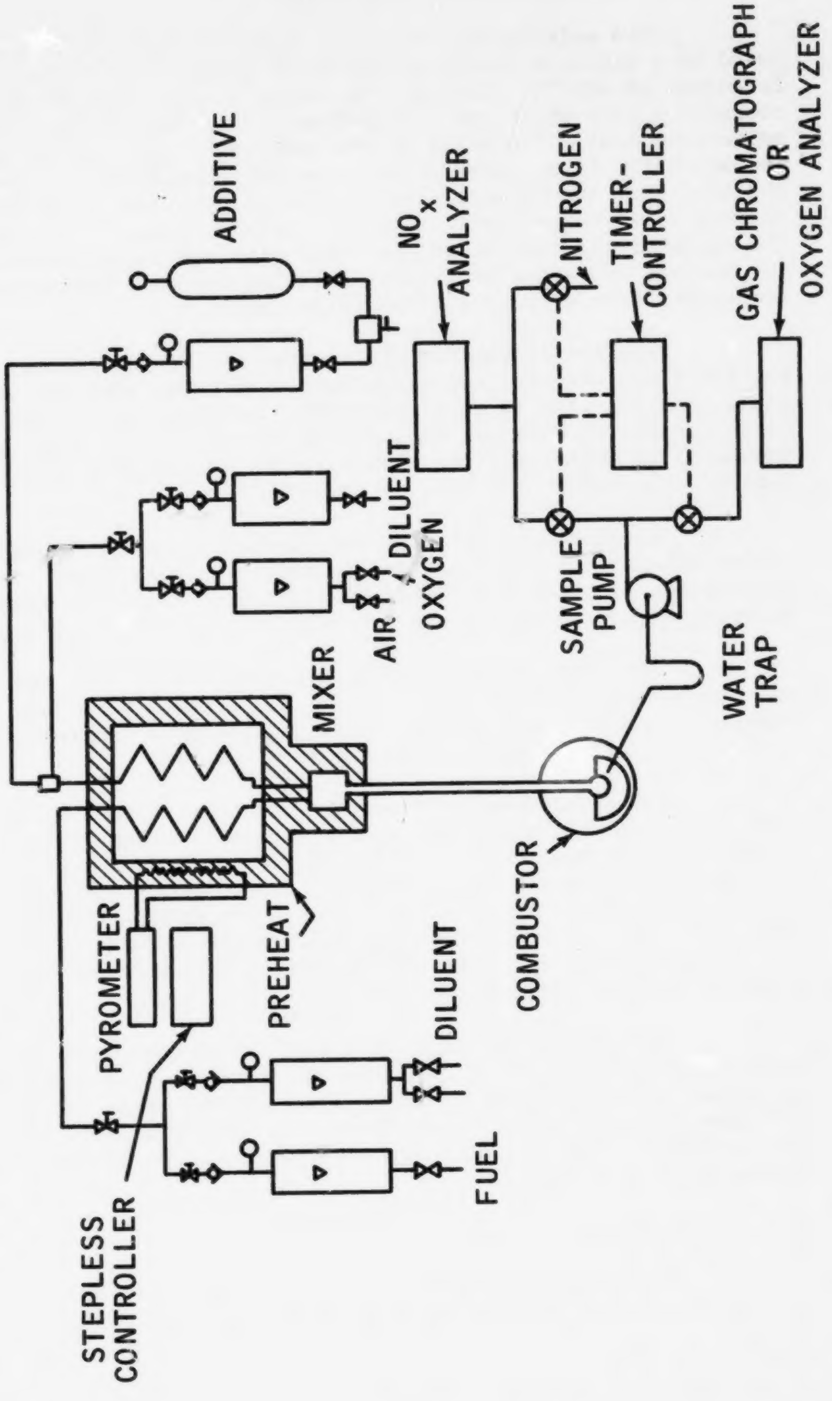

THERMOCOUPLE
PRE-MIXED AIR AND FUEL INLET
INCONEL SPHERE
FIRE BRICK
INJECTOR
FIRE-BRICK
EXHAUST PORT
WATER-COOLED PROBE

Figure 2-1
JET-STIRRED COMBUSTOR

Figure 2-2


ADDITIVE
NO_x ANALYZER
NITROGEN
TIMER-CONTROLLER
GAS CHROMATOGRAPH OR OXYGEN ANALYZER
AIR
DILUENT
OXYGEN
SAMPLE PUMP
WATER TRAP
MIXER
COMBUSTOR
PREHEAT
PYROMETER
DILUENT
STEPLESS CONTROLLER
FUEL

2.1.2 Features of the Multiburner

The multiburner, which is shown schematically in Figure 2-3, is based on a zirconia furnace* capable of being fired to temperatures well in excess of 4000°F. Through the center of this furnace passes a zirconia combustion tube which can be fired upward or downward with gas, oil or pulverized coal. The walls of the combustion tube can be maintained at the adiabatic flame temperature or at any desired wall temperature within the limits of the materials, with control provided by natural gas-oxygen torches fired tangentially into the furnace, external to the combustion tube. The walls of the furnace are provided with two burner ports for these torches and two sight holes for measuring the wall temperature of the combustion tube with an optical pyrometer.

The top of the furnace is designed in two pieces, the lid and the top plug. The lid serves primarily as a gas seal and holds the top plug. The top plug is interchangeable with the bottom plug and contains ports for the furnace gas exhaust and the combustion inlet (when firing downward) or outlet (firing upward). The bottom plug also contains a port for the combustion tube inlet or outlet.

The torches that fire the furnace are water-cooled as are the copper exhaust ducts of the furnace and combustion tube. The exhaust from the furnace is mixed with large quantities of room air, passed through a water spray and vented to the exhaust duct in the furnace enclosure.

The gases are metered with rotameters on both the furnace torches and the combustor tube burner. Flows are controlled by the use of pressure regulators and control valves. This permits good control of the conditions both inside the combustion tube and at its walls.

The multiburner can operate with the combustion zone wall temperature at any desired level and at the extremes it can either be used to remove a large amount of heat from the combustion zone or, if desired, can be used to add heat to the combustion zone. Thus, the multiburner can operate with all of the flexibility of a laboratory combustor without the high heat loss generally found in small-scale devices. This permits the use of the multiburner under combustion conditions that would not be possible with the typical small-scale combustor.

The combustion gases were sampled through water-cooled stainless steel sampling probes** 0.250 inches in diameter with 0.040 inch sampling orifices. One probe was 17 inches long and the other was 25 inches long, and they could be moved along the axis of the combustion tube by a mechanical actuator. The actuation was designed to allow modification for radial motion at a later time.

2.2 Gas Analysis

The techniques selected and developed for combustion gas analysis for the laboratory program have performed satisfactorily and are described below.

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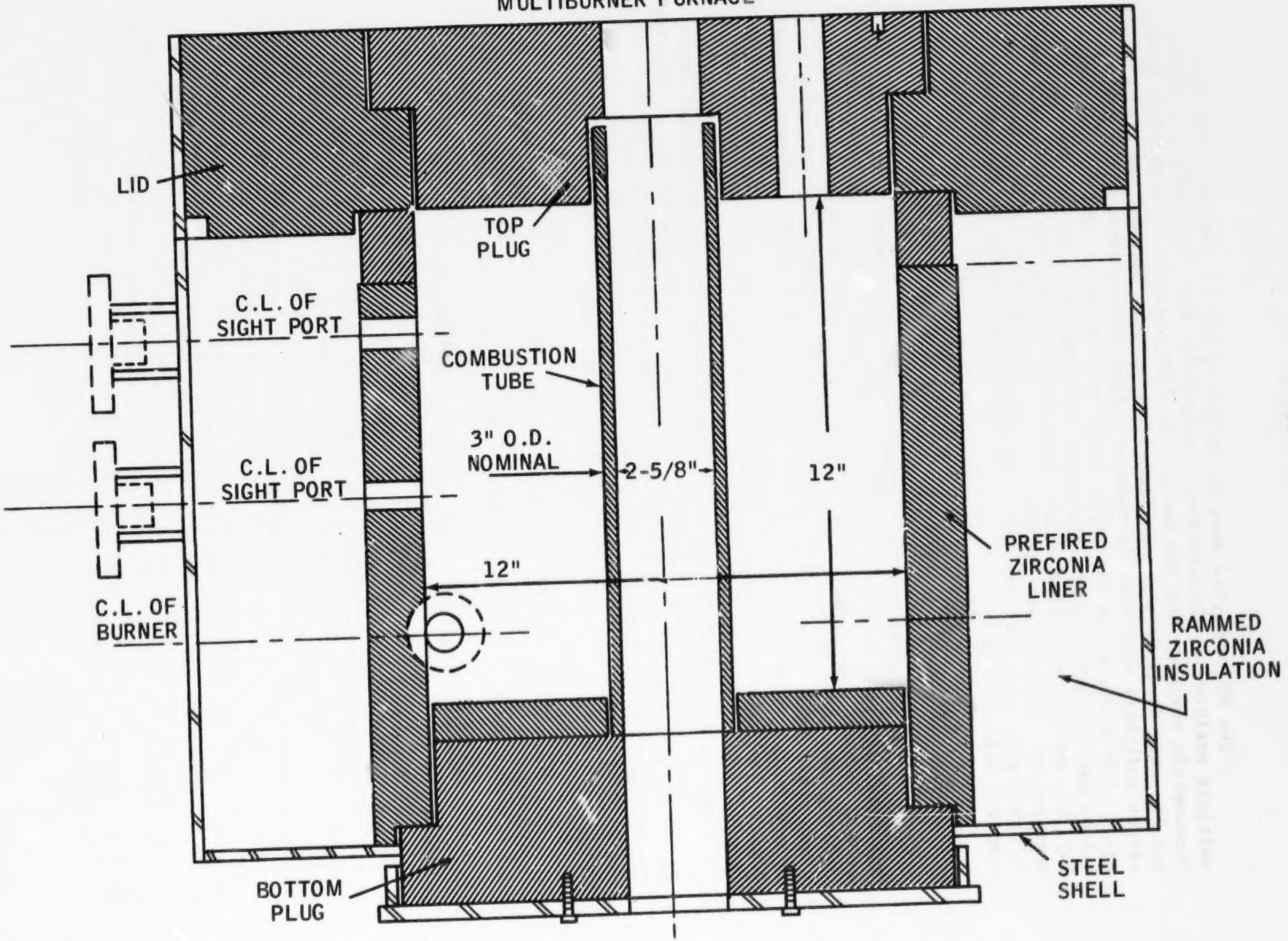
* The zirconia refractory and assistance in the design of the furnace were supplied by Zirconium Corporation of America, Solon, Ohio. The furnace was fabricated to our specifications by C-M Inc., Bloomfield, New Jersey.

** Supplied by Science Products, Dover, New Jersey.

Figure 2-3

MULTIBURNER FURNACE


LID
TOP PLUG
C.L. OF SIGHT PORT
COMBUSTION TUBE
3" O.D. NOMINAL
2-5/8"
12"
C.L. OF SIGHT PORT
12"
PREFIRED ZIRCONIA LINER
C.L. OF BURNER
RAMMED ZIRCONIA INSULATION
BOTTOM PLUG
STEEL SHELL

The NO_x analyses were performed by use of the Envirometrics multigas analyzers. Satisfactory cross-checks were made with the DuPont photometric analyzer and the Beckman NDIR NO analyzer on combustion gases, but the main tools were the Envirometrics units. Two Beckman paramagnetic oxygen analyzers were used to measure oxygen concentration; one has a range of 0-5% O_2, while the other could measure up to 100% O_2. A dual column gas chromatographic separation technique was used for N_2, O_2, CO, CO_2, H_2, and low molecular weight hydrocarbons. Hydrogen could also be measured by utilizing the response of the NO_2 Faristor to H_2. Water could be calculated from both the C/H ratio and the N/O ratio in the outlet compared with the inlet.

2.2.1 Oxides of Nitrogen

The measurements for NO, NO_2, and SO_2 were made with Envirometrics Multigas Analyzers with Faristor plug-in sensors. These analyzers were chosen because they promised "SO_2 selectivity in the presence of nitrogen oxides; NO_2 selectivity in the presence of SO_2 or NO; non-responsive to other prime pollutants." The claims were not found to be uniformly supported by our tests, since the SO_2 Faristor was found to respond to NO_2, the NO_2 Faristor was found to respond to hydrogen and the NO Faristor was found to respond to CO in the range of concentrations that could exist in some of our experiments. Fortunately, with considerable effort and careful attention, these interferences could either be used to good advantage, corrected for by cross-calculation or eliminated by special sampling techniques. The NO/NO_2 measurements are described in this section while SO_2 measurements are briefly discussed in the next section.

The NO/NO_2 measurements were made with Envirometrics analyzers equipped with Faristor detectors. The detectors used were the N76H2 which responded to NO, NO_2, and SO_2, and the N46H2 which responded to NO_2.

The N76H2 was found to have relative sensitivities of about 1.0:0.8:1.0 to NO, NO_2, and SO_2 respectively. The detector could be used easily from 2 ppm NO to concentrations in excess of 3000 ppm. Since our laboratory experiments did not involve sulfur compounds, the response of the N76H2 to SO_2 did not require correction in this case. However, when the analyzer was used in power plant tests where SO_2 was present, the correction was made as required. The response time for the N76H2 to 90% of the steady state value was found to be 5-10 seconds for NO and 20-30 seconds for NO_2. An interference from CO was found in our experiments even though the relative response to CO is less than 10^{-3}. In general, this is not a problem in large boilers where the CO is not allowed to go as high as 1000 ppm. However, in the case of fuel rich combustion, CO levels can easily reach the 1-10% range. Since this is 10,000-100,000 ppm, a 10^{-3} sensitivity will still result in 10-100 ppm equivalent NO. While the sensitivity to CO is less than 10^{-3}, nonetheless attempting to measure 10 ppm or less of NO in the presence of up to 10% CO can present formidable problems.

Fortunately, the response time to CO is much longer than that to NO. In fact, the response to CO follows a complex response curve which ultimately reaches steady state. The sensitivity to CO depends on the past exposure of the detector to CO; after the initial response, the longer the exposure the lower the sensitivity. Indeed, at early times in the hysteresis pattern the response continues to increase for some time even when the cell is purged with zero gas.

The slow response and slow recovery from CO exposure were used to advantage to separate the response to NO_x from the response to CO. The method developed involves the use of sample/purge cycle in which the baseline is checked periodically and the NO_x readings are referenced to this determined baseline. The validity of this method was checked over a wide variety of conditions, with a conditioned Faristor against an NO detector which was not affected by the presence of CO and it was found to be accurate even under conditions where there was only 25-30 ppm NO present at a CO concentration of 10% (100,000 ppm). Since there are unique characteristics of the sensor/analyzer combinations to the presence of CO, each must be checked for sensitivity and response times of possible interference gases.

The use of the Faristor to measure NO_x was checked against the Beckman NDIR in the Esso mobile van while testing a utility boiler and against a DuPont 461 NO_x analyzer in laboratory experiments. The agreement in comparison with the NDIR instrument was good, whether the SO_2 was scrubbed out or not. In the case where SO_2 was not scrubbed, correction for its presence was made by using the response of the S64H2 Faristor which measured SO_2. There was no significant quantity of NO_2 present in these tests. The agreement in comparison with the DuPont analyzer was also good and validated the cyclic sampling technique to eliminate the CO interference. The DuPont had the advantage of eliminating many of the interferences which can affect the Envirometrics under fuel rich conditions and permits continuous analysis for NO_2 (and SO_2 if modified). However, it also has the disadvantage of a long cycle time for analysis of NO (greater than five minutes for NO concentrations in the neighborhood of 100 ppm). At the longer cycle times a peculiar gradual drop off in signal was observed after peak concentrations were reached. This may have been caused by a leak in one of the rotating valves in the system since the analysis for NO is done at approximately five atmospheres pressure. However, there was no way to check for this possibility on the instrument that was used in this study. The drop-off in signal was not rapid enough to cause a major error during the normal five minute cycle of the instrument (perhaps 2 or 3%).

Even with the limitations mentioned, the DuPont instrument performed quite dependably and appeared to be a rugged instrument. Because of the techniques used for analysis of NO, and the resulting long analysis time, the instrument is more suited to industrial monitoring than it is for laboratory investigations of NO formation. Since the instrument was designed with the former purpose in mind, this is no way a fault. As mentioned above, the instrument is quite useful for real time laboratory measurements of NO_2 and with minor filter changes can be used for measuring SO_2.

The NO_2 measurements were made with the N46H2 Faristor which could measure NO_2 from about 2 ppm up. The manufacturer indicates the detector can be used up to 20,000 ppm but these levels were never approached in our tests. This Faristor was generally non-responsive to interference gases, although some of the units developed a gradual negative response to SO_2 which could not be eliminated. However, two gases which were present under fuel rich conditions were found to give a negative response. Hydrogen gave a rapid negative response with a sensitivity of about 2×10^{-4} relative to NO_2 while CO gave a slow negative response of about 2×10^{-5} in one minute, and about 8×10^{-5} in six minutes. The negative response to hydrogen allowed an estimation of hydrogen content of combustion gases on the fuel rich side (the accuracy of this estimate, however, would be only to the nearest percent). Since NO_2 is generally not found on the fuel rich side and since H_2 and CO are not present in significant quantities on the lean side, the NO_2 measurements were not affected by the presence of H_2 and CO.

2.2.2 Sulfur Dioxide

For measurements of SO_2 we have an S64H2 Faristor for use in the Envirometrics analyzer. The detector responds to SO_2 but also responds to NO_2 in a negative manner by 100-150%. In most combustion applications the NO_2 emissions are small and thus would not present a serious problem, but for cases where NO_2 levels are high, a correction for the presence of NO_2 must be made. The S64H2 Faristor was not used in the laboratory for SO_2 measurements since sulfur was not included in our study, but it was used on an emergency basis to measure NO_2 when the N46H2 Faristor was out of service. The S64H2 was used in connection with the boiler test program to measure NO_x in the presence of SO_2 and the net NO_x measurements were in good agreement with NDIR measurements for NO.

2.2.3 Oxygen

The oxygen analysis was made with a Beckman paramagentic oxygen analyzer (described here) and by gas chromatography (described in the next section). The Beckman oxygen analyzer measures the net magnetic effect produced by the gas sample in the analysis cell. Oxygen is paramagnetic, while most of the background gases are slightly diamagnetic. The major exception is NO which is also paramagnetic and produces a positive interference equivalent to 44% of its concentration. Since the oxygen measurements were made to the nearest 0.1% (1000 ppm) this correction is not important at NO concentrations below 1000 ppm. The diamagnetic species produce a negative response but the major background gas present was nitrogen and the calibrations were made with a nitrogen background gas so corrections during a run did not become significant.

The minor nature of the interferences other than nitric oxide is indicated below:

Gas	Response produced by Pure Gas at One Atmosphere Pressure, %
N_2	-0.36
CO	-0.35
CO_2	-0.63
H_2	-0.12
CH_4	-0.36
C_2H_6	-0.82
O_2	+100.00

Care was taken when using the paramagnetic oxygen analyzer to avoid water condensation in the instrument, and measurements were taken with little or no flow through the instrument to avoid adverse effects on the test body and quartz fiber in the analyzer section. Most of the measurements were made with the model C2 which measured 0-5% O_2, but higher levels were measured with the model E2 which was capable of measuring up to 100% O_2.

2.2.4 Gas Chromatography for Major Gas Components

A dual-column chromatographic separation technique was used to measure N_2, O_2, CO, CO_2 and hydrogen and hydrocarbons when present. Although the technique is capable of separating NO and NO_2 as well, the concentrations of these species were generally not high enough to permit accurate measurements.

The two chromatographic columns were placed in series, the first column consisting of one-eighth inch stainless steel tubing packed with six feet of Poropak Q followed by two inches of Poropak R, porous polyaromatic polymer gel. The second column consisted of one-quarter inch stainless steel tubing packed with six feet of 5A molecular sieve. Column 1 was used primarily for CO_2 although it was also capable of separating C_2H_6 and NO_2, while Column 2 was used primarily for O_2, N_2, CO, H_2 and CH_4, and was also capable of resolving NO. The compressed air used in our experiments was quite low in argon content (typically 450 ppm) and therefore the presence of this gas did not interfere with the chromatographic analysis for oxygen.

2.2.5 Hydrogen

In addition to chromatographic separation, it was possible to analyze for hydrogen using the Envirometrics Analyzers. It was found that the N46H2 Faristor would respond in a negative direction on the fuel rich side when burning hydrocarbons or hydrogen as fuel. By checking possible interference gases it was established that the major interfering gas was hydrogen. Since NO_2 was not present on the fuel rich side, it was possible to use this interference to obtain an approximate hydrogen concentration. While the sensitivity was generally low (about 2×10^{-4} which is 2 ppm NO_2 equivalent for each percent hydrogen) the output of the N46H2 Faristor was high enough and steady enough when in good condition to give a reproducible result on a strip chart recorder.

2.2.6 Water

Since we were using cooled sampling probes and since we also cooled the sample gas to about a 40°F dew point, it was not possible to continuously analyze for water content. However, the water content could be determined in one of two ways. Using an oxygen balance the nitrogen/oxygen ratio in the input gas (from air) could be compared with the nitrogen/oxygen ratio in the output gas (nitrogen from molecular nitrogen and oxygen from molecular oxygen, CO and CO_2; neglecting the contribution of nitrogen oxides), and the difference could be attributed to water. A second method involved a hydrogen balance comparing the carbon/hydrogen ratio from the input gases (hydrocarbons) with the carbon/hydrogen ratio in the output gases (carbon from carbon monoxide, carbon dioxide and unburned hydrocarbons and hydrogen from molecular hydrogen and hydrocarbons). The missing hydrogen in the output was attributed to water. These two methods generally gave fairly good agreement (within 0.5% absolute concentration) but were , of course, dependent on the accuracy of the measurements for carbon, hydrogen, oxygen, and nitrogen.

2.3 Experimental Results*

The jet-stirred combustor, based on the original design of Longwell and Weiss (2-5) has been used to determine the amount of NO_x found in hydrocarbon oxidation under intensely back-mixed and kinetically limited conditions. Because of the intense back-mixing prevailing in the jet-stirred combustor, mass, energy and momentum transport limitations are kept at a minimum. Thus, this combustor permits the investigation of combustion phenomena controlled by the chemical kinetics of the process.

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* Detailed data tabulations are presented in Appendix A.

Most of our work in the jet-stirred combustor was carried out with methane as the fuel. Additional experiments were run with hydrogen, carbon monoxide, and propane fuels.* Concentrations of NO_x and other combustion gas species were measured by direct probing of the combustor with water-cooled probes, and combustion temperature measurements were made with thermocouples. A broad range of fuel/air mixture ratios were investigated, and NO_x concentration measurements were made using Envirometrics Faristors and validated by comparison with measurements using a DuPont NO/NO_2 spectrophotometric analyzer. Simple bond-type additives were introduced at known concentration levels, and the NO_2 concentrations thus observed were compared with base-line data obtained in the absence of additives.

A "multiburner" unit capable of burning gas, oil and coal on a laboratory scale has been installed in our laboratories. In initial experiments, the multiburner has been operated as a "slice" of a large furnace by heating the walls of the combustion tube and firing a premixed methane air mixture into the tube. The effects of residence time, mixture ratio, and wall temperature have been investigated. The unit has proven its durability in successive cycles of testing.

2.3.1 Effect of Mixture Ratio on NO_x Formation in Jet-Stirred Combustor

The formation of NO_x in combustion has been studied in the jet-stirred combustor for a variety of fuels over a wide range of mixture ratios. The fuels used were methane, hydrogen, carbon monoxide and propane. The well-stirred nature of the jet-stirred combustor with nearly instantaneous mixing of reactants with products provides an almost uniform, intense flame zone with the resultant distribution of reactants, intermediates and products. NO_x concentrations were considerably higher than those predicted by application of Zeldovich kinetics assuming oxygen atoms to be in equilibrium with dissociating molecular oxygen and peak NO_x emissions were found to occur on the fuel-rich side. This could be caused by a combination of two factors:

(1) Oxygen atom "overshoot" can occur in hydrocarbon flames during the chain branching sequence and at least a portion of the species in the reaction zone of the jet-stirred combustor is undergoing this portion of reaction sequence.

(2) Because of the intense backmixing in the jet-stirred combustor, the combustion zone always contains a certain fraction of reactants, and therefore, molecular oxygen is present, evern under fuel-rich conditions.

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* Typical compositions of fuel gases are given in Appendix B.

The NO_x formation in the combustion of methane/air mixtures at constant residence time are shown in Figure 2-4. The preheat temperature was 375°F, but the substantial heat losses reduce the reaction temperature below that for adiabatic combustion. The variation in mixture ratios was achieved by holding the air flow constant and varying the fuel flow. Since, for methane, at stoichiometric conditions the air flow on a volume basis is approximately ten times the fuel flow, variation in mixture ratio from 70% to 200% stoichiometric air results in a variation in total mass flow rate of only ± 5%. Each air flow rate used was characterized by a "nominal residence time" which is calculated by dividing the reactor volume by the volumetric flow rate at stoichiometric conditions taking measured temperature into account.

The peak NO_x emissions occur at approximately 90% stoichiometric air, and the agreement between the measurements taken with the Envirometric analyzer and those taken with a Dupont Model 461 photometric analyzer show good agreement. The results are reported in volumetric parts per million, as measured. The measurements were taken with water removed from the gas to a dew point of 40°F so that water would not condense in the analyzers. A slight change in the appearance of the curve would occur if the results were corrected to a given fuel flow rate, but the curve is so steep that this change would not be major.

The variation in the NO_x emissions with nominal residence time is shown in Figure 2-5. Within experimental error it appears that there is no significant different in measured NO_x with residence time. However, in Figure 2-6 it can be seen that there are substantial differences in temperatures[b] with residence time caused by the higher heat losses at longer residence times. If it is assumed that residence time (within the range of experiment) has little effect on the controlling species, calculations indicate that an activation energy between 50 and 85 Kcal (average close to 75 Kcal) for the controlling process would result in the observed relative behavior. If the controlling process is indeed the reaction

$$O + N_2 = NO + N$$

as might be expected, then the levels of NO produced in the jet-stirred combustor could only be explained by "super-equilibrium" oxygen atom concentrations[a]. Calculations using equilibrium concentrations of oxygen atoms result in substantially lower NO_x emissions than observed. However, we note that the hypothesis of super-equilibrium oxygen atom concentrations by no means eliminates other possibilities.

(a) Super-equilibrium oxygen atom concentration defined as greater than that corresponding to the equilibrium $O_2 + M = 2O + M$ at the prevailing O_2 concentration.

(b) The temperatures indicated in Figure 2-6 are not gas phase temperatures but reference temperatures taken in the vicinity of the wall. It is likely that this temperature varies in the same manner as the gas phase temperature.

Figure 2-4

NO_x EMISSIONS IN JET-STIRRED COMBUSTOR

METHANE-AIR

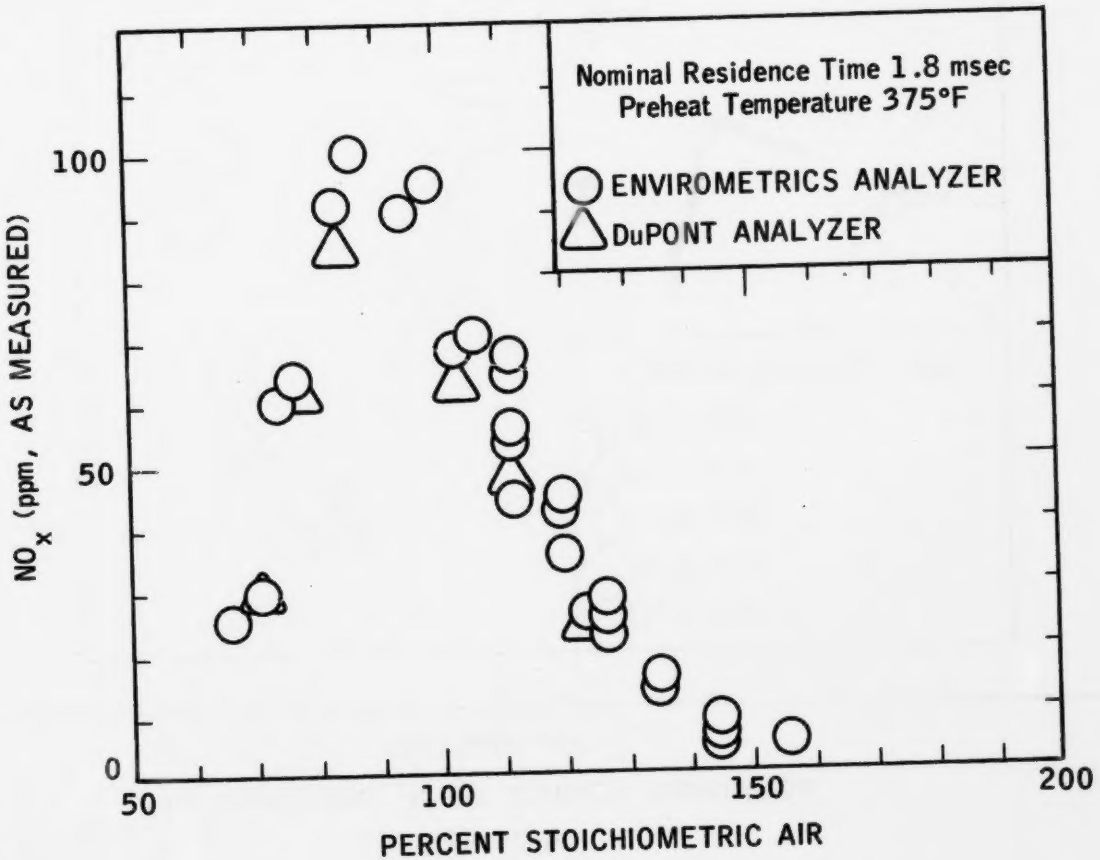


Figure 2-5

NO_x EMISSIONS IN JET-STIRRED COMBUSTOR

METHANE-AIR

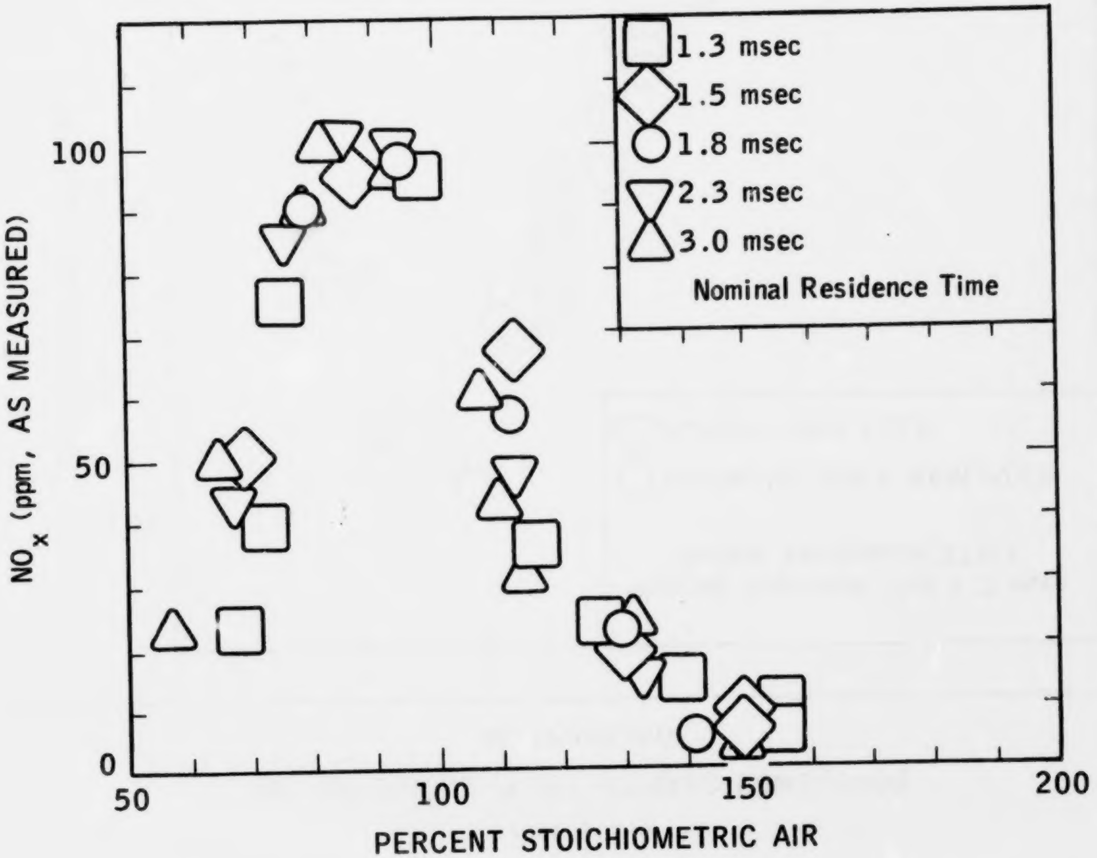
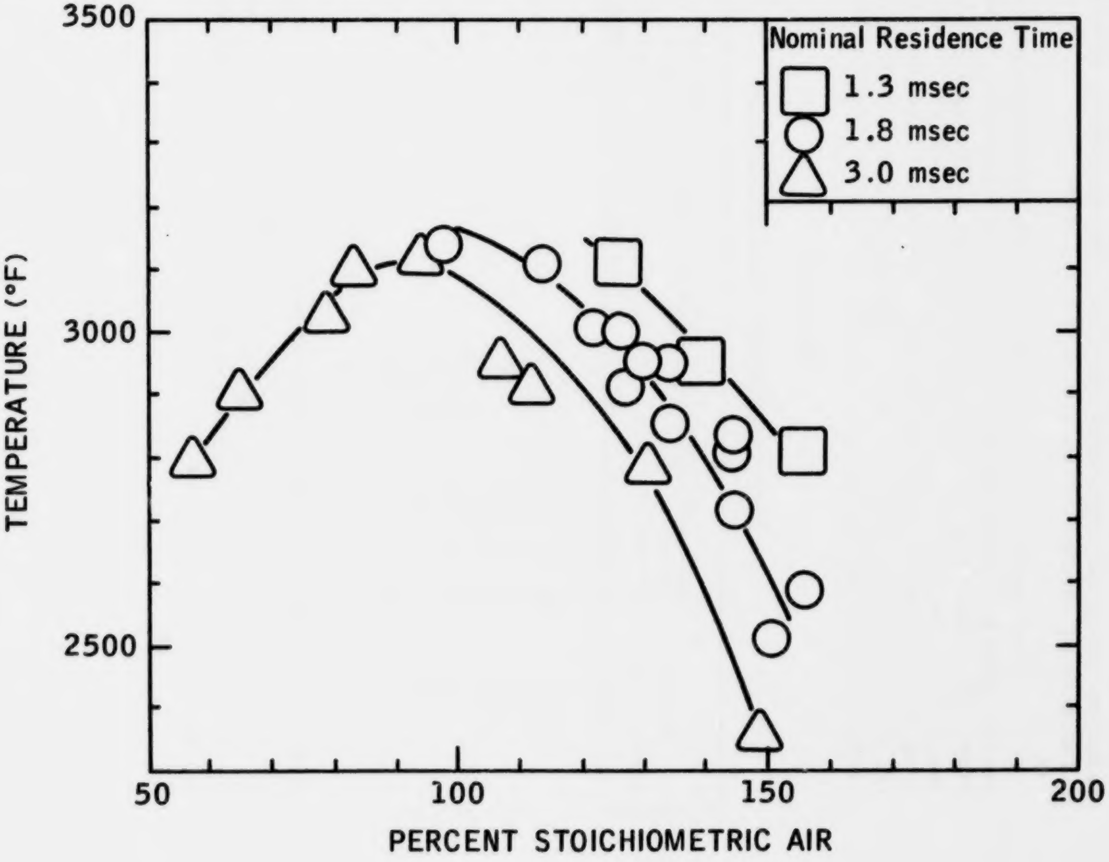


Figure 2-6

TEMPERATURE VS. MIXTURE RATIO IN JET-STIRRED COMBUSTOR



The molecular oxygen concentrations measured in the jet-stirred combustor under fuel-lean conditions fall quite close to the levels expected for complete combustion. However, below stoichiometric air, because of the intense backmixing, oxygen levels are still measurable. While the absolute differences are small under fuel-rich conditions, the relative differences on the fuel-rich side can be substantial in a back-mixed reactor when compared to a plug flow reactor where the reaction can go to completion rapidly. The measured oxygen levels as a function of mixture ratio are shown in Figure 2-7.

The combustion gases were analyzed chromatographically for carbon dioxide carbon monoxide, methane and hydrogen. It was determined after the data had been obtained that a non-reproducible air leak occurred at the sampling valve which prevented accurate chromatographic determination of nitrogen and oxygen. Therefore, the results for CO_2, CO, CH_4 and H_2 are reported on a relative basis in Table 2-1. The carbon containing species are reported on a mole fraction basis as the fraction of total carbon. The hydrogen is reported as a molar ratio to the total carbon in the sample. Thus,if one takes this information together with the mixture ratio and oxygen measurements obtained independently the total stable gas distribution can be calculated. The overall stoichiometry of methane/air combustion is

Table 2-1

Measured Exhaust Gas Distribution

Percent Stoichiometric Air	Carbon Distribution			Molecular Hydrogen (Molar ratio to Total Carbon)	Molecular Oxygen (Percent of Exhaust, Dry Basis)
	Carbon Dioxide Fraction	Carbon Monoxide Fraction	Methane Fraction		
145	0.991	0.009	--	--	7.1
127	0.982	0.018	--	--	5.5
112	0.946	0.054	--	--	2.6
101	0.855	0.145	--	--	1.0
92	0.741	0.259	--	--	0.4
84	0.644	0.356	--	0.28	0.3
77	0.519	0.481	--	0.59	0.3
71.5	0.365	0.635	--	0.74	0.2
66	0.259	0.534	0.207	0.38	3.9

$$CH_4 + 2\chi\, O_2 + 7.52\chi\, N_2 \longrightarrow$$

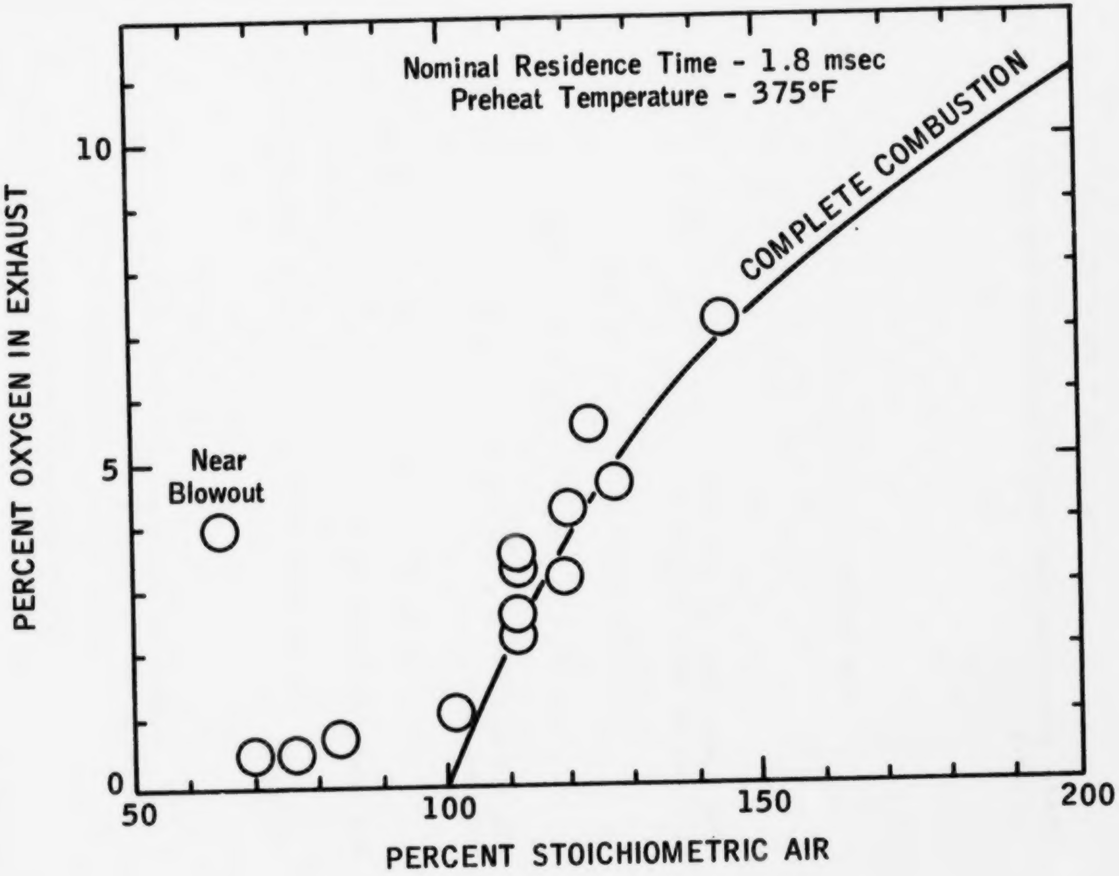
$$(A)\ CO_2 + (B)\ CO + (C)\ CH_4 + (D)\ H_2 + (E)\ O_2 +$$

$$(F)\ H_2O + (G)\ N_2 \qquad (2\text{-}1)$$

where χ is the fraction of stoichiometric air in the feed gas and (A) through (G) are the stoichiometric coefficients of the products.

Figure 2-7

PERCENT OXYGEN VS. MIXTURE RATIO
JET-STIRRED COMBUSTOR - METHANE/AIR



The carbon balance is as follows

$$(A) + (B) + (C) = 1 \tag{2-2}$$

These quantities have been measured and are given in the required form in Table 2-1.

The hydrogen balance is as follows

$$(C) + \frac{(D)}{2} + \frac{(F)}{2} = 1 \tag{2-3}$$

The quantities (C) and (D) can be found in Table 2-1 and the quantity (F) can be calculated from equation 2-3.

The oxygen balance is as follows

$$(A) + \frac{(B)}{2} + (E) + \frac{(F)}{2} = 2\chi \tag{2-4}$$

The quantities (A), (B) and χ are in Table 2-1, and (E) can be calculated from

$$(\%\ O_2\ \text{dry}) = \frac{(E)}{(A) + (B) + (C) + (D) + (E) + (G)} \tag{2-5}$$

and equation (2-4) can be used as a cross-check of the value of (F).

The nitrogen balance (neglecting the contribution of fixed nitrogen) is

$$(G) = 7.52\chi \tag{2-6}$$

When the coefficients (A)-(G) are determined the overall gas composition can be obtained from

$$\frac{(M)}{(A) + (B) + (C) + (D) + (E) + (F) + (G)} \tag{2-7}$$

where (M) represents any of the coefficients (A)-(G). The results of these calculations are shown in Table 2-2.

TABLE 2-2

CALCULATED EXHAUST GAS COMPOSITION (WET BASIS)

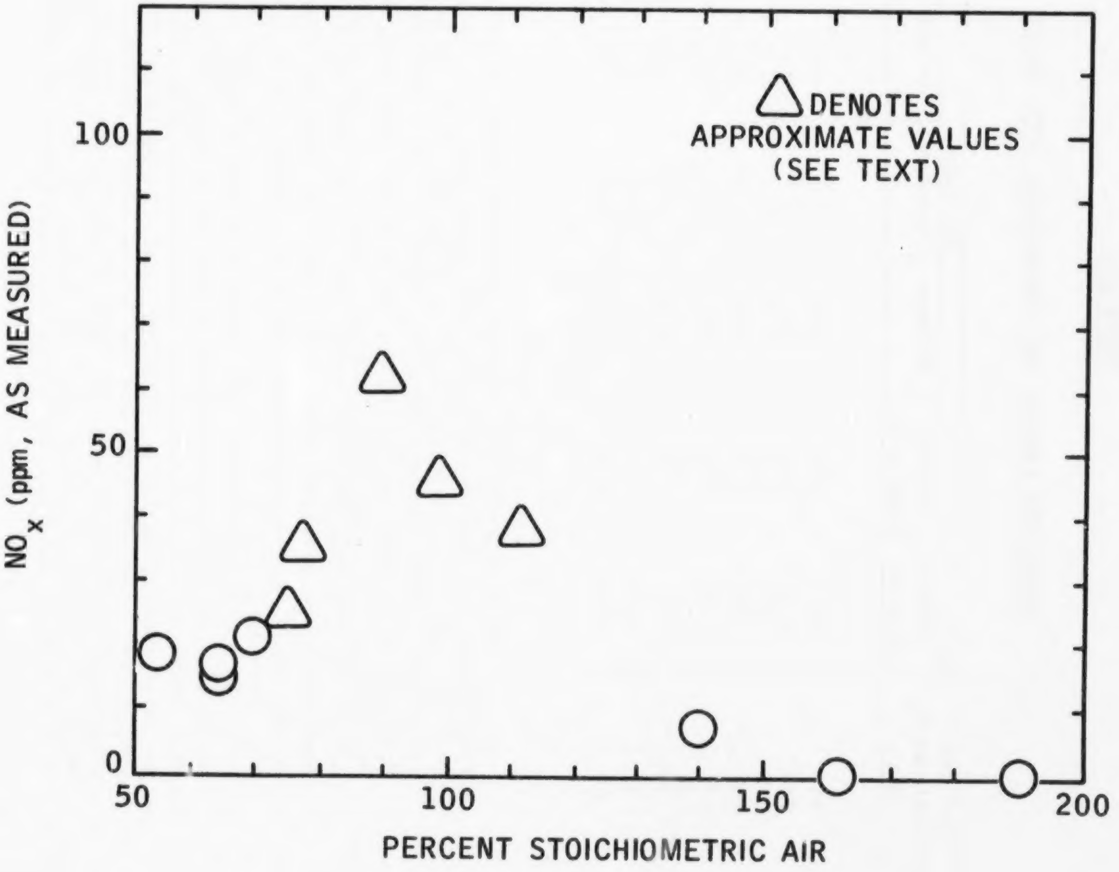
Per Cent Stoichiometric Air	Per Cent						
	Carbon Dioxide	Carbon Monoxide	Methane	Hydrogen	Oxygen	Water	Nitrogen
145	6.7	0.1	0.0	0.0	6.1	13.5	73.6
127	7.5	0.1	0.0	0.0	4.7	15.2	72.5
112	8.1	0.5	0.0	0.0	2.2	17.1	72.1
101	8.0	1.4	0.0	0.0	0.8	18.7	71.1
92	7.4	2.6	0.0	0.0	0.3	20.1	69.5
84	6.9	3.8	0.0	3.0	0.2	18.1	67.9
77	5.9	5.4	0.0	6.7	0.2	16.5	65.3
71.5	4.3	7.5	0.0	8.7	0.2	16.0	63.3
66	3.3	6.9	2.7	4.9	3.1	14.9	64.1

When hydrogen was used as the fuel in the jet-stirred combustor, substantially higher temperatures were developed. In fact, the temperatures were so high that the fuel and air preheat had to be essentially eliminated to prevent damage to the combustor. Even so, the temperatures for hydrogen-air combustion were about 300°F hotter than those for methane-air combustion. Despite the higher temperatures, the measured NO_x output was considerably lower than that for the methane-air case. Peak emissions occurred under fuel-rich conditions and essentially no NO_x could be measured above 150% stoichiometric air. The results are shown in Figure 2-8. It will be noted that the symbols between 75% and 120% stoichiometric air are shown as broken symbols. Between these mixture ratios, the temperatures in the jet-stirred combustor were well above 3300°F, and therefore, the combustor could not be held at these conditions for a sufficient time to completely assure steady conditions. The combustor was run for as long as practical at these conditions, and an estimate was made of the steady NO_x value that would be reached, based on previous experience with the combustor. The broken symbols indicate the element of uncertainty for these points; about

Figure 2-8

NO_x EMISSIONS IN JET-STIRRED COMBUSTOR

HYDROGEN-AIR



20% for all such data points, except at 90% stoichiometric air where the uncertainty is estimated at 40%. The lower NO_x concentrations at higher temperatures are unexpected if one assumes the same controlling reactions for NO_x formation in methane and hydrogen combustion.

Two possibilities may explain this phenomenon. One is that the oxygen atom concentration may not be at equilibrium for hydrocarbon combustion in the jet-stirred combustor. This is quite reasonable based on previous observations and calculations on NO_x formation in combustion. Furthermore, as noted above, to calculate the observed NO_x formation in methane combustion, assuming it is controlled by the reactions

$$N_2 + O = NO + N$$

$$O_2 + N = NO + O$$

substantial "super-equilibrium" concentrations of oxygen atoms would be required. The second possibility is that hydrocarbons or other carbonaceous species may be participating in NO_x formation. This could be a direct participation between carbonaceous species and nitrogenous species to produce other intermediates easily oxidized to NO, or it could be an interaction between carbon-containing species and oxygen-containing species to produce high oxygen atom concentrations. The latter interaction actually combines both possibilities discussed by requiring the participation of carbon-containing species in the production of super-equilibrium oxygen atom concentrations. These inferences based on experimental evidence require verification based on detailed calculations and analysis of the elementary reactions involved. Good evidence has been uncovered in this study for significant coupling between the hydrocarbon combustion reactions and NO formation reactions in a backmixed reactor. Further evidence results from our study of carbon monoxide combustion.

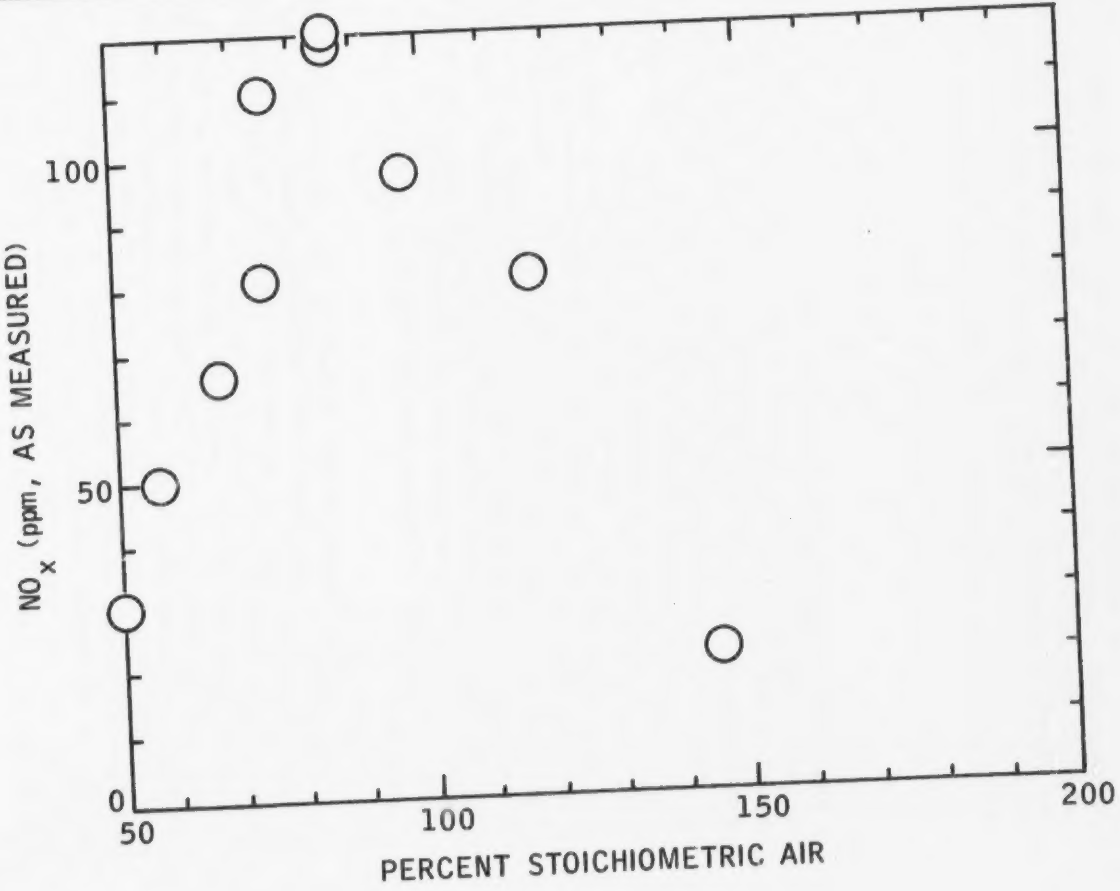
Carbon monoxide was burned in the jet-stirred combustor with air. Actually it was found that Technical Grade carbon monoxide could be burned without special attention, but C.P. Grade required very small additions of hydrogen to burn successfully. Thus, it is likely that the Technical Grade CO itself contained small amounts of hydrogen. Consequently, in all the CO runs, both hydrogen and carbon were present even though the amount of hydrogen was quite small. The temperatures for CO combustion were higher than those for methane (about 200° F), but lower than those for hydrogen. The NO_x emissions were higher in CO combustion than in either methane or hydrogen combustion, as shown in Figure 2-9. Peak emissions are found on the fuel-rich side. Once more, the levels attained cannot be explained by Zeldovich kinetics with "equilibrium" oxygen atom concentrations.

Several experiments were performed to attempt to further determine the role of the fuel type in NO_x formation in the jet-stirred combustor. Small amounts of methane or carbon monoxide were added to hydrogen in a number of the runs. Mixture ratios were selected where the differences between the fuels were most definitive and the curves

Figure 2-9

NO_x EMISSIONS IN JET-STIRRED COMBUSTOR

CARBON MONOXIDE-AIR



could be distinguished. Considerations was given to the uncertainty of the data for hydrogen between 70 and 130% stoichiometric air. The results were as follows: For hydrogen combustion with methane comprising five mole percent of the fuel mixture (equivalent to 17% of fuel stoichiometry) the NO_x emissions were 45 ppm for the mixture, where they had been 61 ppm for methane and 32 ppm for hydrogen; they were 30 ppm for the mixture, where they had been 42 ppm for methane and 25 ppm for hydrogen. For a 50:50 carbon monoxide-hydrogen mix the NO_x emissions were 90 ppm (85% stoichiometric air), where they were 50 ppm for hydrogen and 120 ppm for carbon monoxide. For a mixture of primarily carbon monoxide with 10% hydrogen, the emissions were 62 ppm (70% stoichiometric air), where they were 20 ppm for hydrogen and they were 64 ppm for carbon monoxide; at 132% stoichiometric air the emissions were 42 ppm for the mix, 15 ppm for hydrogen and 40 ppm for carbon monoxide. The results for the mixtures indicate that the input fuel does influence the resulting NO_x emissions in the jet-stirred combustor. Small amounts of hydrogen do not dramatically reduce NO_x emissions in either hydrocarbon or carbon monoxide combustion. Small amounts of CO or methane do not dramtically increase the NO_x emissions from hydrogen combustion. However, there does appear to be an effect of fuel mixtures on NO_x emissions in the jet-stirred combustor. Thus, the coupling of NO_x formation with combustion does not appear to be a catalytic effect, but rather, an overall effect governed by the concentrations of reactants, which in turn govern the controlling intermediates.

The NO_x emissions for propane-air combustion are shown in Figure 2-10. The NO_x levels are essentially indistinguishable from the carbon monoxide results, even though the measured temperatures are considerably lower. As was found with methane, hydrogen and carbon monoxide, peak NO_x emissions occur under slightly fuel-rich conditions. The NO_x emissions are higher than those predicted from the Zeldovich mechanism with "equilibrium" oxygen atoms, and the NO_x levels are slightly higher than those for methane combustion, even though the temperatures are roughly comparable. Temperature measurements(a) for propane are shown in Figure 2-11.

2.3.2 Effect of Added Nitrogen Compounds on NO_x Formation in the Jet-Stirred Combustor

A number of experiments have been performed in which simple, model nitrogen-containing compounds have been added to the reaction zone of the jet-stirred combustor during the combustion of methane. The compounds used represent either fuel nitrogen bond-types or potential nitrogenous intermediates in the flame zone. These experiments were not designed to be either an exhaustive study of fuel compounds or of nitrogen bond-types themselves. The purpose of this set of experiments was to investigate the nature and behavior of the nitric oxide formation reactions involving nitrogen compounds differing substantially in bond types. Compounds were chosen to illustrate the difference as simply as possible. Nitrogen-oxygen, nitrogen-hydrogen and nitrogen-carbon bonds were used in the study. The compounds selected were nitric oxide

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(a) These are reference temperatures as described for the case of methane.

Figure 2-10

NO_x EMISSIONS IN JET-STIRRED COMBUSTOR

PROPANE-AIR

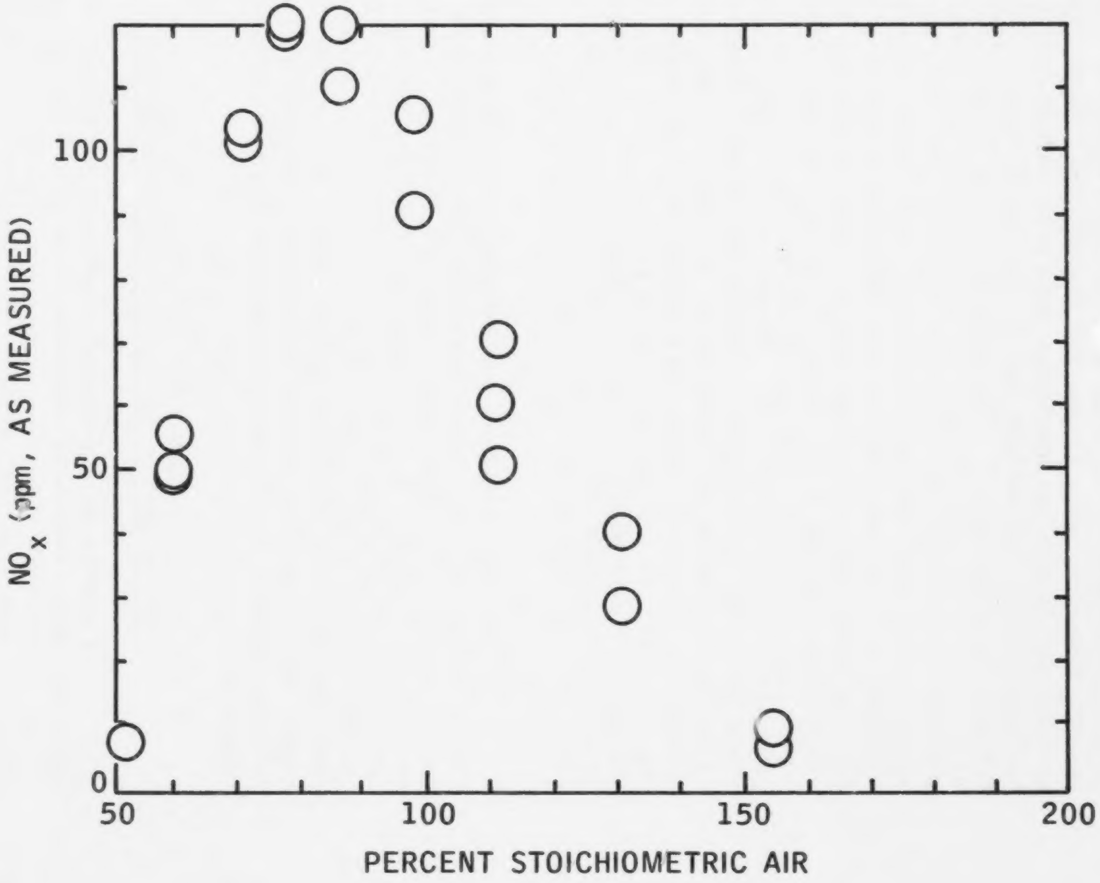
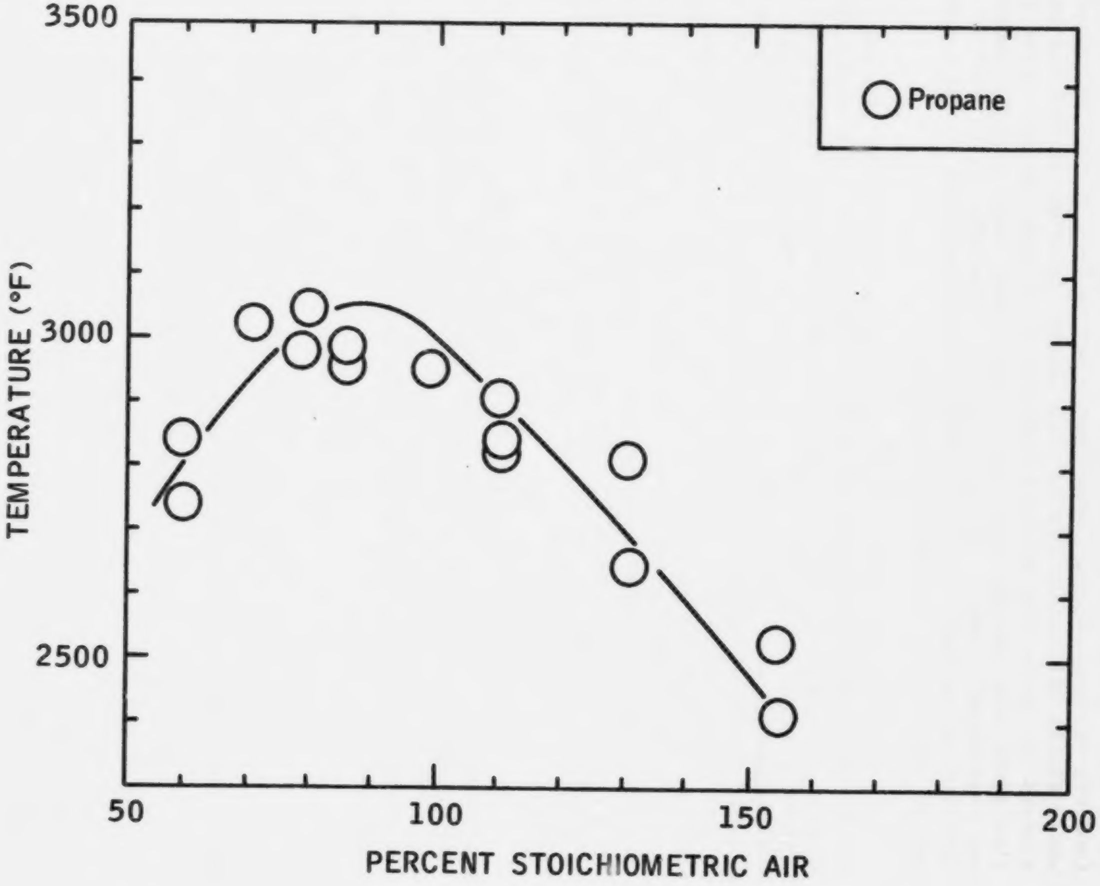


Figure 2-11

TEMPERATURE VS. MIXTURE RATIO IN JET-STIRRED COMBUSTOR



and nitrogen dioxide for nitrogen-oxygen; ammonia for nitrogen-hydrogen; cyanogen for nitrogen-carbon. Methylamine was used for a carbon-nitrogen-hydrogen bond combination. The experimental results indicate that the oxidation of bound nitrogen can be essentially quantitative even at the short residence times (ca. 2 msec) in the jet-stirred combustor. Differences were found in the production of nitric oxide from the various nitrogen bond types ranging from 60 to 100% conversion under excess air conditions, but the general behavior of all the compounds studied was quite similar as a function of mixture ratio. Under fuel rich conditions the production of nitric oxide from nitrogen compounds was considerably lower, approaching zero below 60% stoichiometric air. The fate of the portion of the additive not resulting in NO_x formation was not determined in these experiments.

The retention of nitric oxide as a function of mixture ratio in the jet-stirred combustor burning methane/air is shown in Figure 2-12. There is essentially total retention on the fuel lean side, but the retention drops off on the fuel rich side, approaching zero below 60% stoichiometric air. The degree of retention is found to be independent of additive level up to almost 3000 ppm equivalent addition. The change in NO_x output for the jet-stirred combustor as a function of additive input is illustrated in Figure 2-13. The equivalent addition of NO_x has been corrected for the removal of water from the sampled stream; the change in NO_x output is based on as measured values with the gas stream at a dew point of 40°F. The nitric oxide results can be regarded as a baseline, since no change in the additive is required to yield the output.

When NO_2 was added to the jet-stirred combustor, a slightly different behavior was observed. The NO_x emission levels were slightly higher and, within a narrow range of mixture ratios, more NO_x was measured in the output than was added initially to the combustor. The significant reactions to produce NO from NO_2 in the jet-stirred combustor are likely to be

$$NO_2 + O = NO + O_2$$

$$NO_2 + M = NO + O + M$$

The latter reaction could be followed by

$$O + N_2 = NO + N$$

$$N + O_2 = NO + O$$

The reaction of nitrogen dioxide with oxygen atoms has a very low activation energy while the dissociation of NO_2 has a fairly high activation energy. Within the range of temperature and concentrations of our experiments it is possible that the dominant reaction for NO_2 shifts from the exchange reaction to the dissociation reaction. If the exchange reaction

$$NO_2 + O = NO + O_2$$

were predominant the NO_2 would be converted to NO with the loss of an oxygen atom. If the dissociation reaction

$$NO_2 + M = NO + O + M$$

Figure 2-12

RETENTION OF ADDED NO

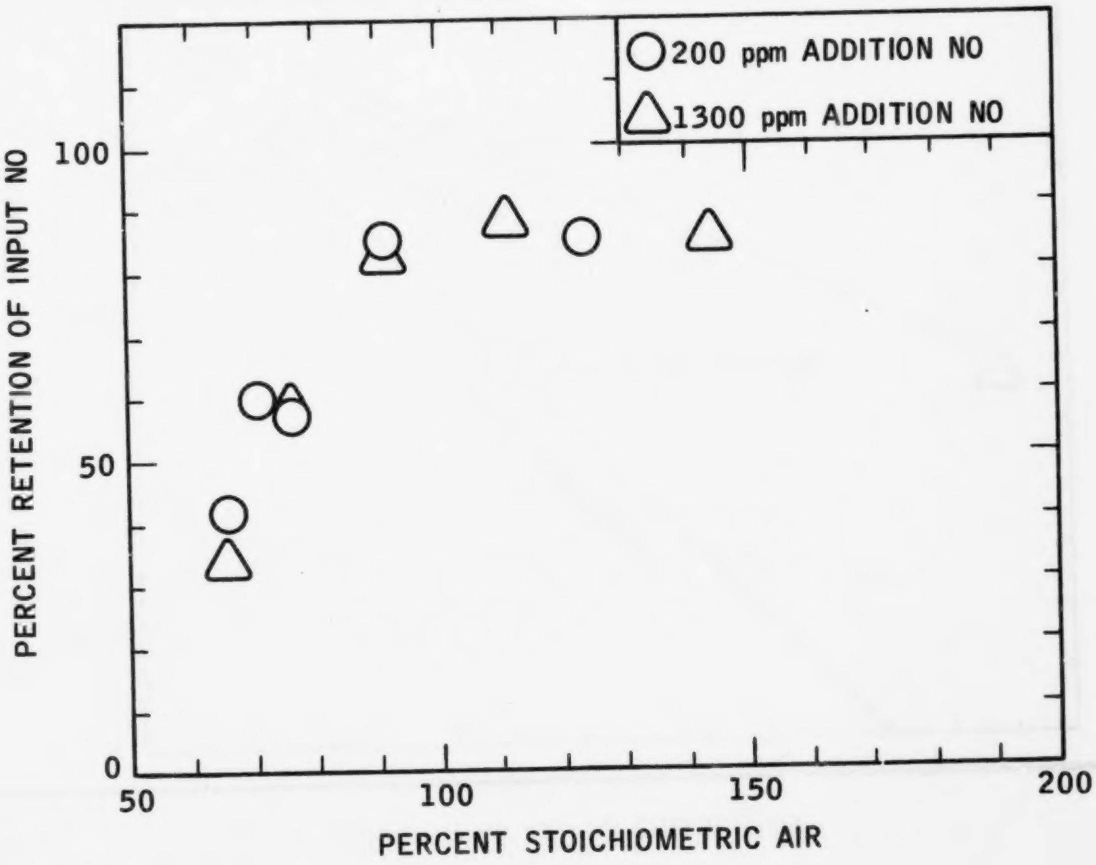
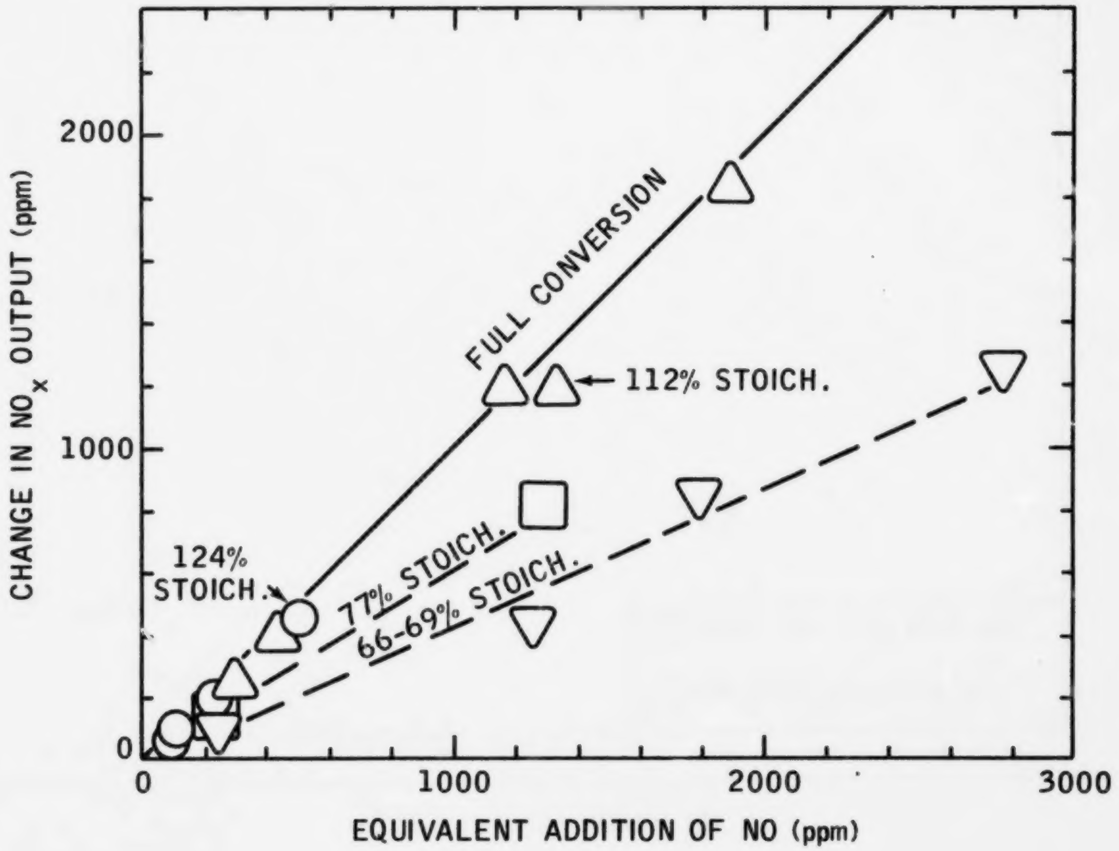


Figure 2-13

ADDITION OF NO TO COMBUSTOR



were predominant NO_2 would be converted to NO with the production of an oxygen atom which itself might react to produce additional NO.

In our experiments (Figure 2-14), it was found that under fuel lean conditions the added NO_2 was quantitatively converted to NO although for a narrow range of mixture ratios (around 110% stoichiometric air) slightly more than quantitative conversion was found. The excess NO_x, however, was small and is barely outside the limits of experimental uncertainty. Under fuel rich conditions, the conversion drops off and approaches zero below 60% stoichiometric air. Full conversion of NO_2 to NO at 124% stoichiometric air is unaffected by additive levels ranging from 100 to 800 ppm as shown in Figure 2-15.

Ammonia (Figure 2-16) gives slightly lower conversions than the oxides of nitrogen themselves but the conversion is still fairly high (ca. 70% under fuel lean conditions). The conversion falls off on the fuel rich side, approaching zero at about 60% stoichiometric air. The general nature of the conversion curve is the same as that for nitric oxide and indicates that conversion of fuel nitrogen to NO_x is reduced under fuel rich conditions much as the NO_x emissions from methane combustion. The conversion of ammonia to nitric oxide as a function of additive level is shown in Figure 2-17 and indicates that the percentage conversion is essentially independent of additive level from 100 ppm up to almost 3000 ppm equivalent addition.

Cyanogen (Figure 2-18) gives the lowest conversion of any of the model nitrogen compounds used in this study. The overall appearance of the conversion curve is quite similar to those for NO and NH_3. With excess air, conversion is essentially constant at about 60%. Under fuel rich conditions the conversion drops off, approaching zero between 60 and 70% stoichiometric air. The conversion of cyanogen to nitric oxide as a function of additive level is shown in Figure 2-19 and again indicates that the percentage conversion is essentially independent of additive level from 100 ppm up to 3000 ppm equivalent addition. Data have been taken at 5000 ppm equivalent addition at 124% stoichiometric air which indicate a slight drop-off in conversion.

Methylamine was also added to the jet-stirred combustor as a model compound with carbon-nitrogen-hydrogen bonding. The percentage conversions to NO_x as a function of mixture ratio are shown in Figure 2-20. The results are almost indistinguishable from those for ammonia except that the conversion approaches zero at about 65% stoichiometric air. The overall conversion under fuel lean conditions is approximately 70%. The conversion of methylamine to NO_x as a function of additive level is shown in Figure 2-21. There is essentially constant conversion at 112% stoichiometric air from 200 to 1200 ppm equivalent addition.

Figure 2-14

CONVERSION OF NO_2 TO NO_x

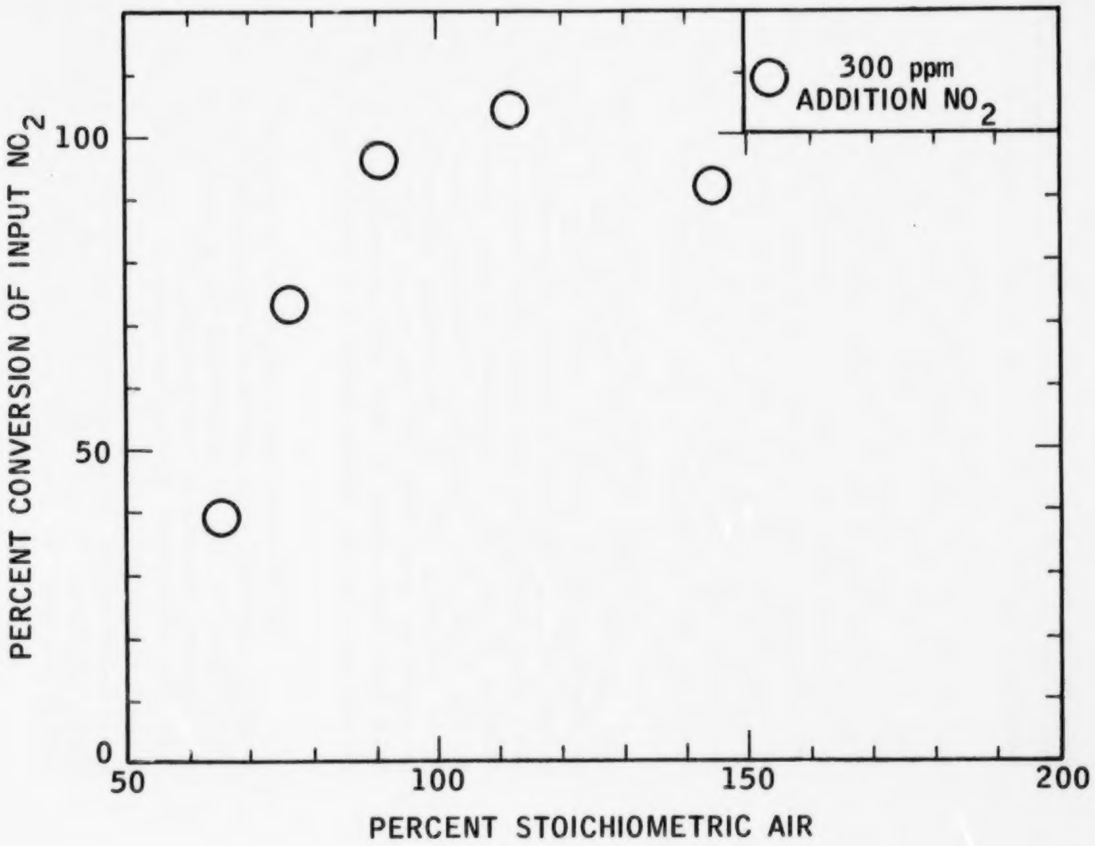


Figure 2-15

ADDITION OF NO_2 TO COMBUSTOR

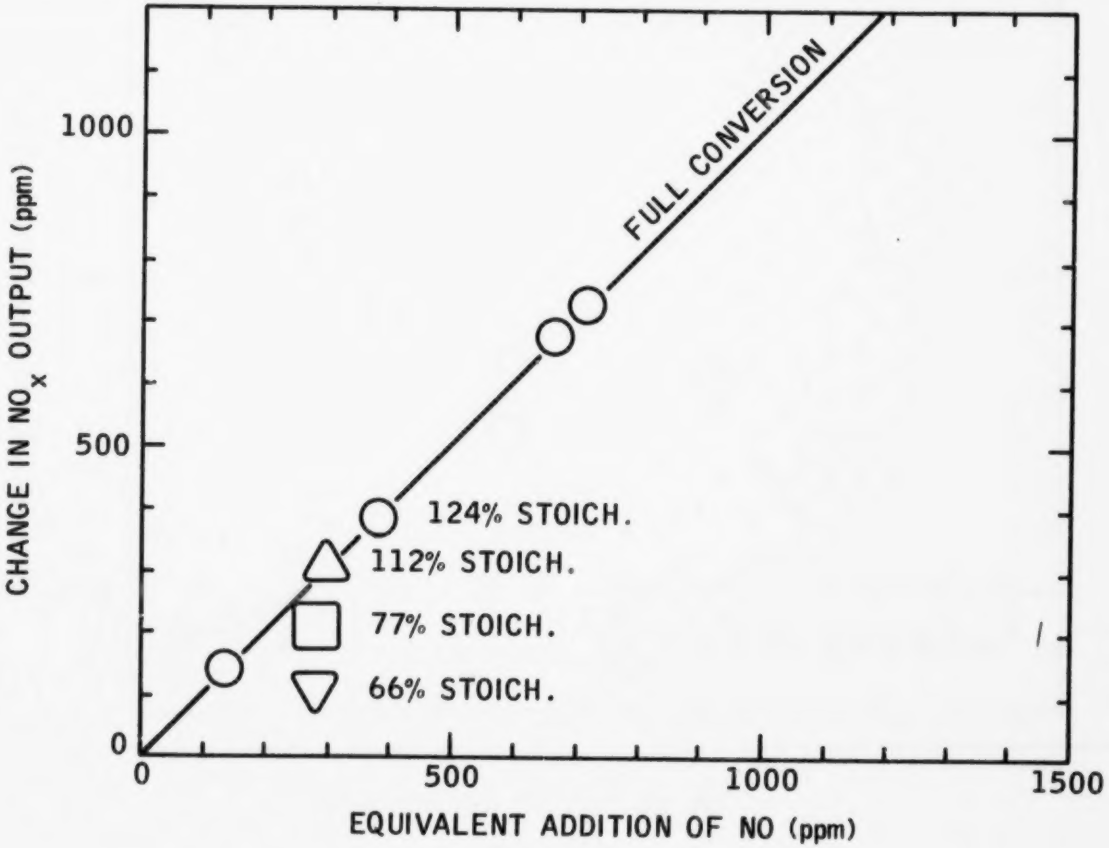


Figure 2-16

CONVERSION OF NH_3 TO NO_x

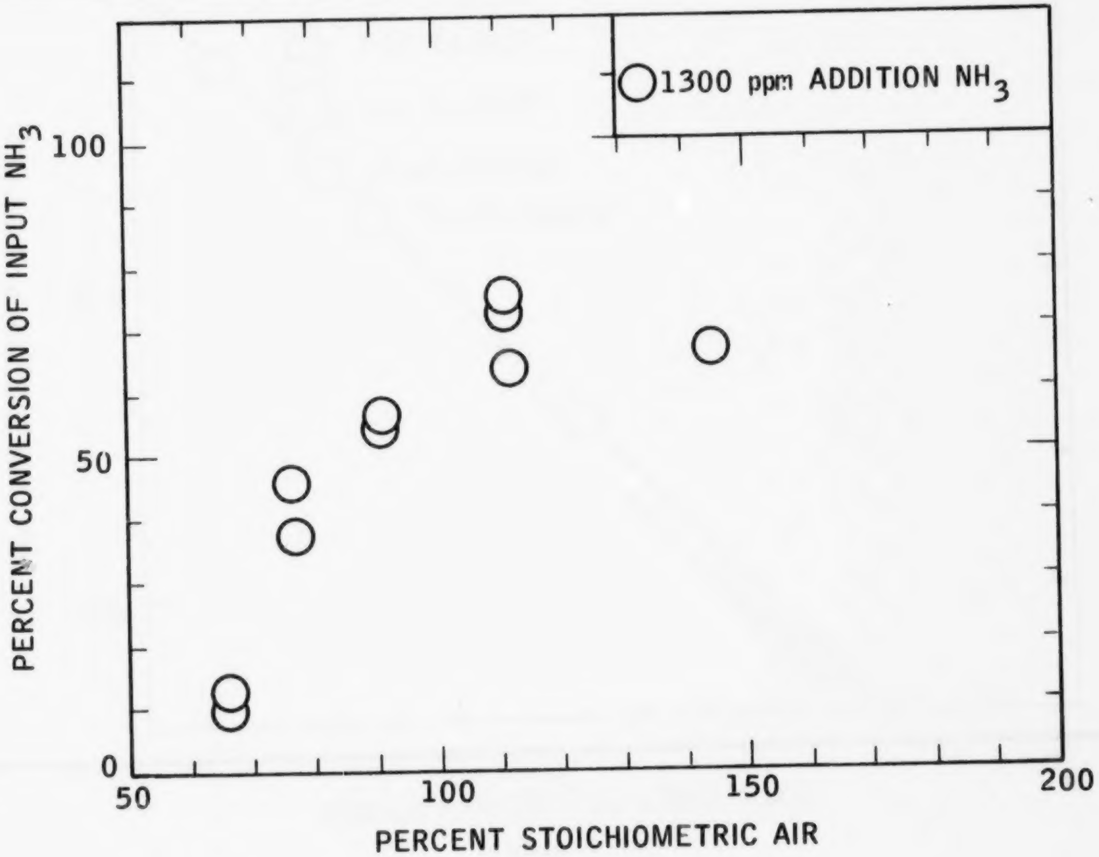


Figure 2-17

ADDITION OF NH_3 TO COMBUSTOR

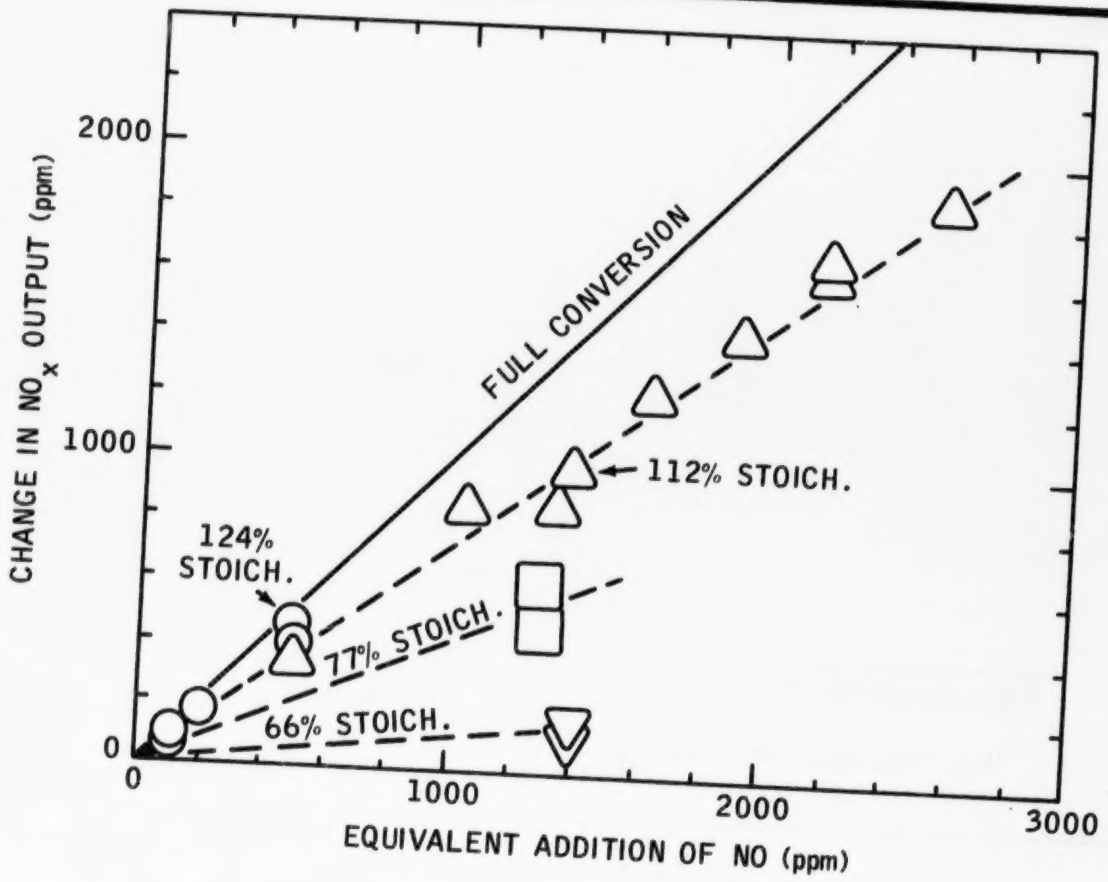


Figure 2-18

CONVERSION OF $(CN)_2$ TO NO_x

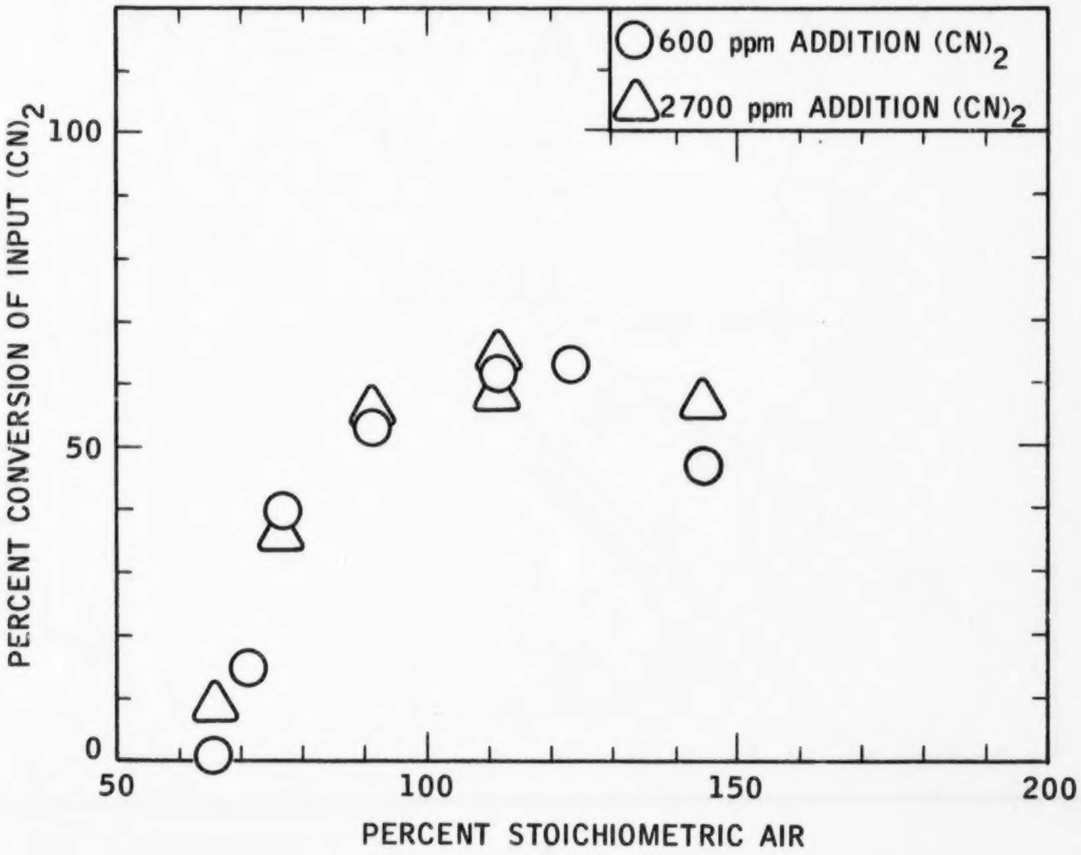


Figure 2-19

ADDITION OF $(CN)_2$ TO COMBUSTOR

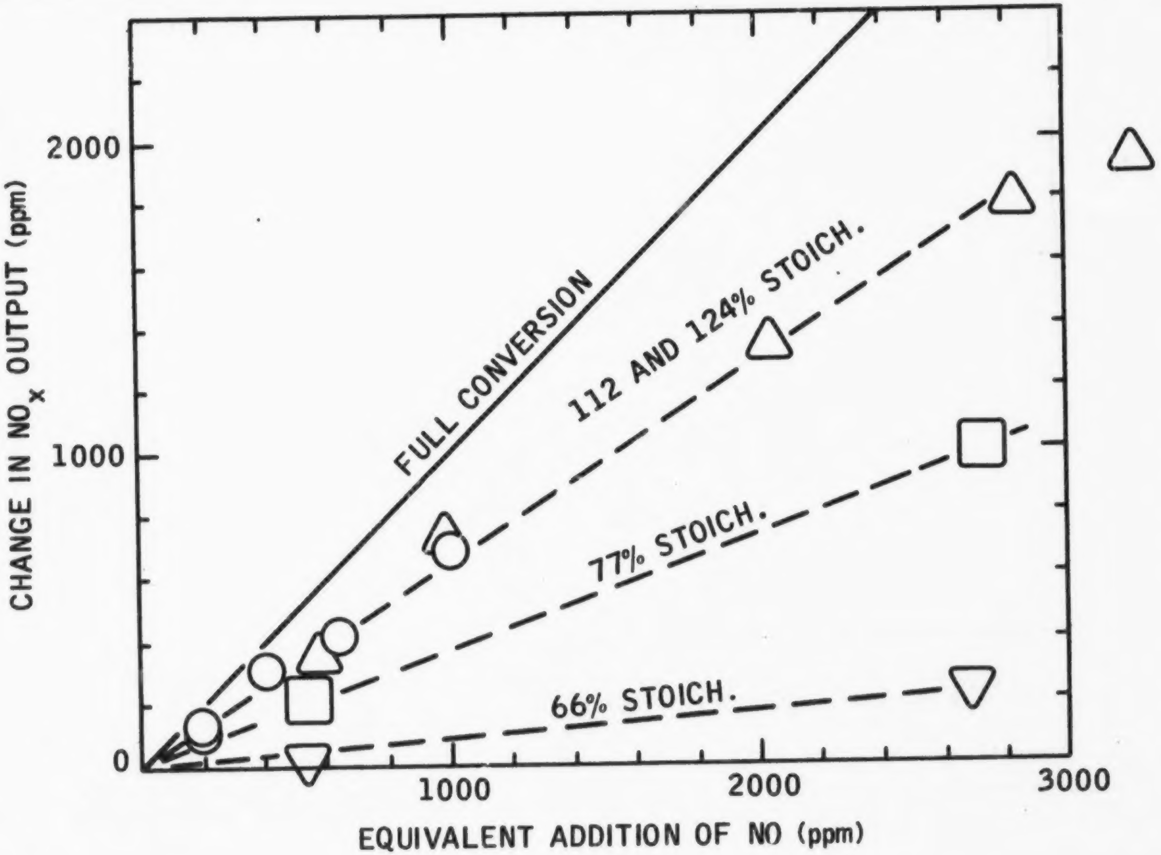


FIGURE 2-6

CONVERSION OF CH_3NH_2 TO NO_x

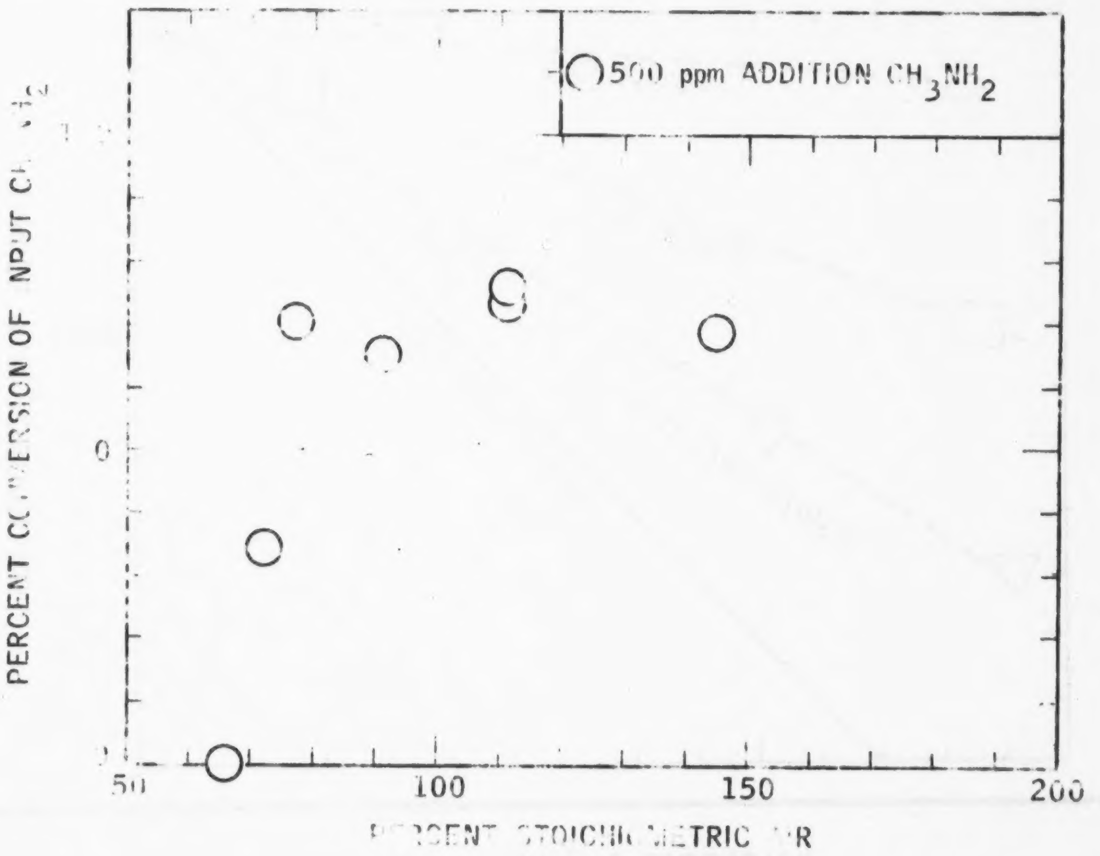
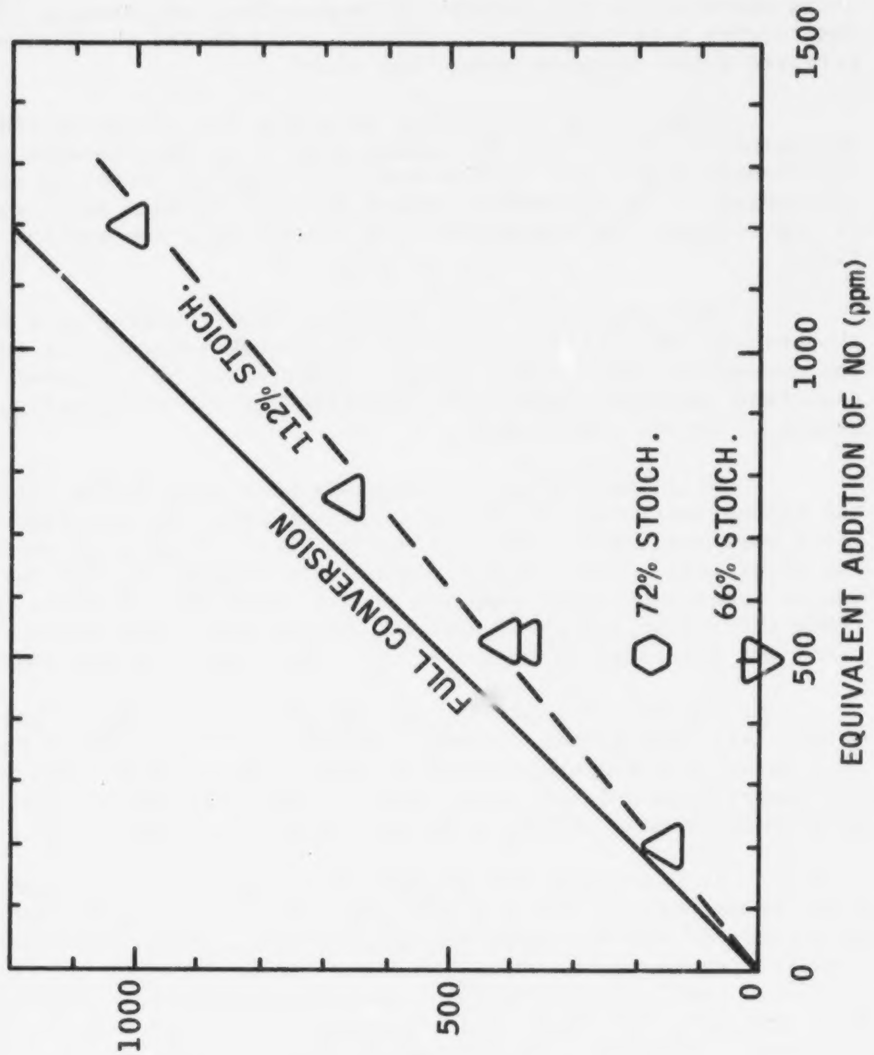


Figure 2-21

ADDITION OF CH_3NH_2 TO COMBUSTOR



2.3.3 Preliminary Observations and Results with Multiburner

The multiburner is a zirconia furnace with a combustion tube running through its center. The furnace is fired with natural gas (or propane)/oxygen torches, and the materials of construction allow operation of the furnace at temperatures approaching 4500°F. The torches fire tangentially through ports in the insulation and the prefired fused zirconia monolithic liner.

Exploratory experiments have been run on the multiburner to determine its durability and flexibility as an experimental tool. The furnace itself was conditioned over numerous cycles to complete the curing of the refractory lining and insulation. After conditioning of the furnace, the combustion tube was put in place and the furnace was fired.

The monolithic liner exhibited some cracking as a result of the heating and cooling cycles but in general retained its integrity. The combustion tube itself, however, fabricated of a thermal shock resistant zirconia composition, exhibited no visible cracking as a result of cyclic operations.

Wall temperature measurements were made on the outer wall of the combustion tube with an optical pyrometer. No temperature measurements were made inside the tube during these preliminary experiments. The gases inside the combustion tube were sampled through the water-cooled, stainless steel sampling probes described earlier. During these initial experiments, only NO_x was measured, although the sampling train was also capable of measuring other combustion gas components.

The formation of NO_x was measured for air alone and for methane/air combustion. During a given set of experiments the combustion tube outer wall temperature was maintained constant and the combustion gas composition and flow rates were varied. The reactor was probed axially to measure the NO_x level at a given position.

It was found that because of the heated walls, combustion could be maintained over a wider range of conditions than otherwise possible. Of course, under extremely fuel rich conditions with wall temperatures above the adiabatic flame temperature one can observe pyrolysis reactions rather than combustion reactions. Excursions were made into this rich region although no analytical measurements were made. Excursions to 20% stoichiometric air at a wall temperature of 2800°F resulted in the formation of large quanitities of soot and second stage burning at the exhaust of the combustion tube.

Experiments were performed in which air was passed into the combustion tube with the outer wall maintained at 3150°F (2000°K). NO_x concentrations were measured along the axis of the tube to measure the effect of residence time; further residence time information was obtained by varying the flow rate. The results for NO_x formation under these conditions are shown in Figure 2-22. The line indicated on the figure is a "best fit" line. The results fall below those calculated by using rate constants for the elementary reactions involved but this is not surprising since in these experiments the gas temperature was probably somewhat below the temperature of the outer wall of the combustion tube. Gas temperature measurements were not made in these experiments but will be performed in future studies. The results are presented here primarily to illustrate the use of this equipment to establish experimental conditions under which significant quantities of NO_x can be produced. In order to properly interpret the results of such experiments a more complete characterization of the flow patterns, temperature distribution and gas compositions must be obtained.

Further experiments were performed to illustrate the use of the multi-burner to study NO_x formation in methane/air combustion. A premixed flame of methane/air was studied over a range of residence times and mixture ratios. To vary mixture ratio, the methane flow was held constant while the air flow was varied. This differs from the procedure used in the jet-stirred combustor. Since the air flow rate is much higher than the methane flow rate this procedure results in residence times which vary with mixture ratio. To graph the resulting data (which were taken at constant fuel rate) a "nominal" residence time was defined as the residence time under stoichiometric conditions at the combustion tube wall temperature.

Under combustion conditions, peak NO_x levels were found to be about 170 ppm. While for pure air under similar residence time and wall temperature conditions the NO_x formation was 30-50 ppm, it is likely that the gas temperatures were different for the combustion cases and the non-combustion cases. With good characterization of temperature and flow conditions it may be possible to measure the contribution of combustion-related reactions to NO_x formation. Residence time seemed to have only a minor effect on peak NO_x formation as illustrated in Figure 2-23. Under excess air conditions the residence time effect seemed to be greater, but the data are not sufficiently extensive to draw firm conclusions on this matter.

Wall temperature, however, was found to have an effect (Figure 2-24). At 3150°F, the NO_x level at 100% stoichiometric air was found to be 175ppm while at 2800°F the NO_x level was 120ppm. This is in directional agreement with the difference between large boilers and laboratory-scale experimental equipment regarding NO_x levels measured. By use of the multiburner the effect of heat losses on NO_x formation can be measured and further information can be obtained on the roles of thermal conditions and chemical conditions in NO_x formation.

Figure 2-22

Preliminary Data

PRODUCTION OF NO_x FROM AIR

IN MULTIBURNER WALL TEMPERATURE 3150°F

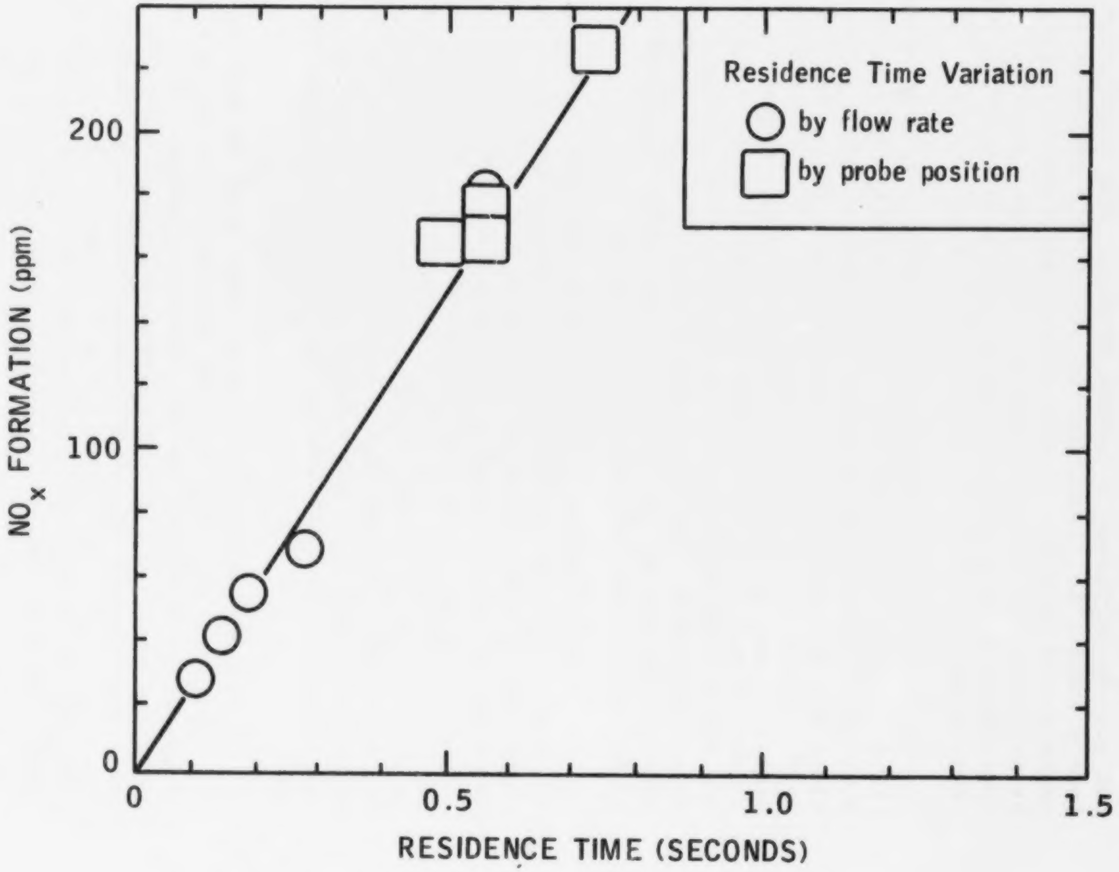


Figure 3-[illegible]

Preliminary Data

EFFECT OF MIXTURE RATIO ON
NO_x FORMATION IN MULTIBURNER

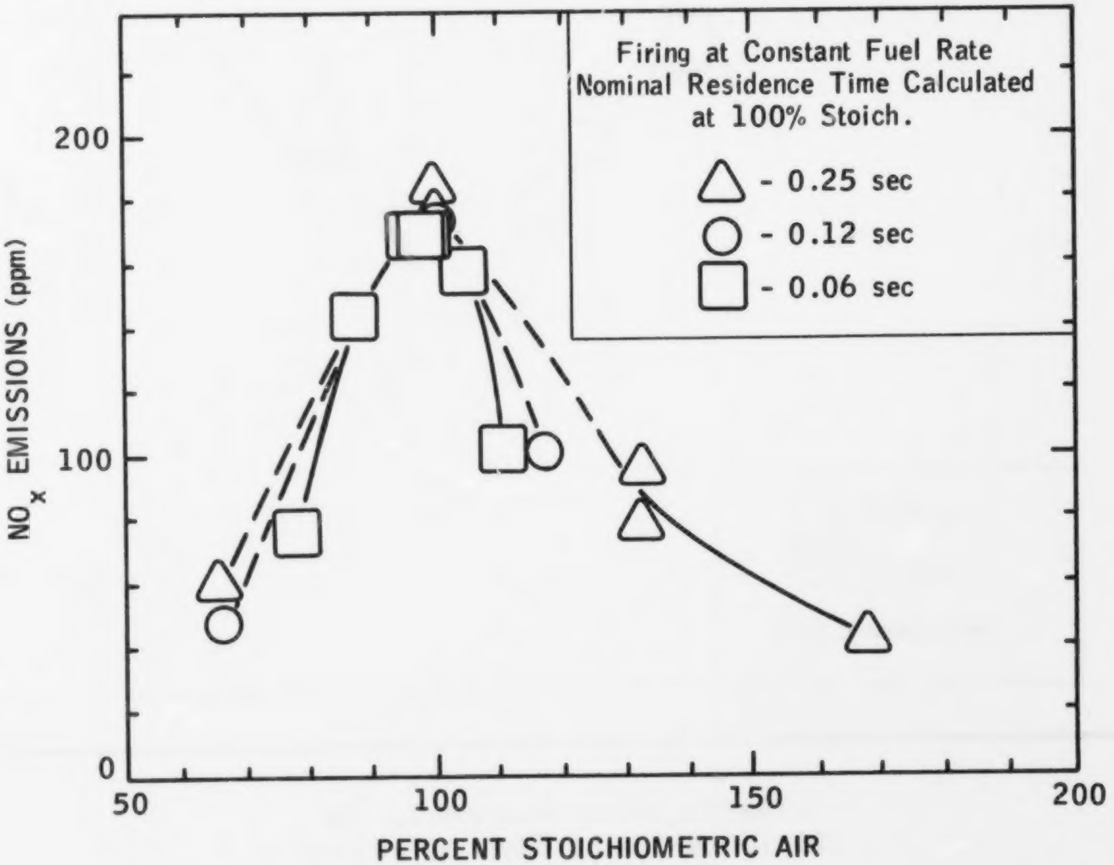
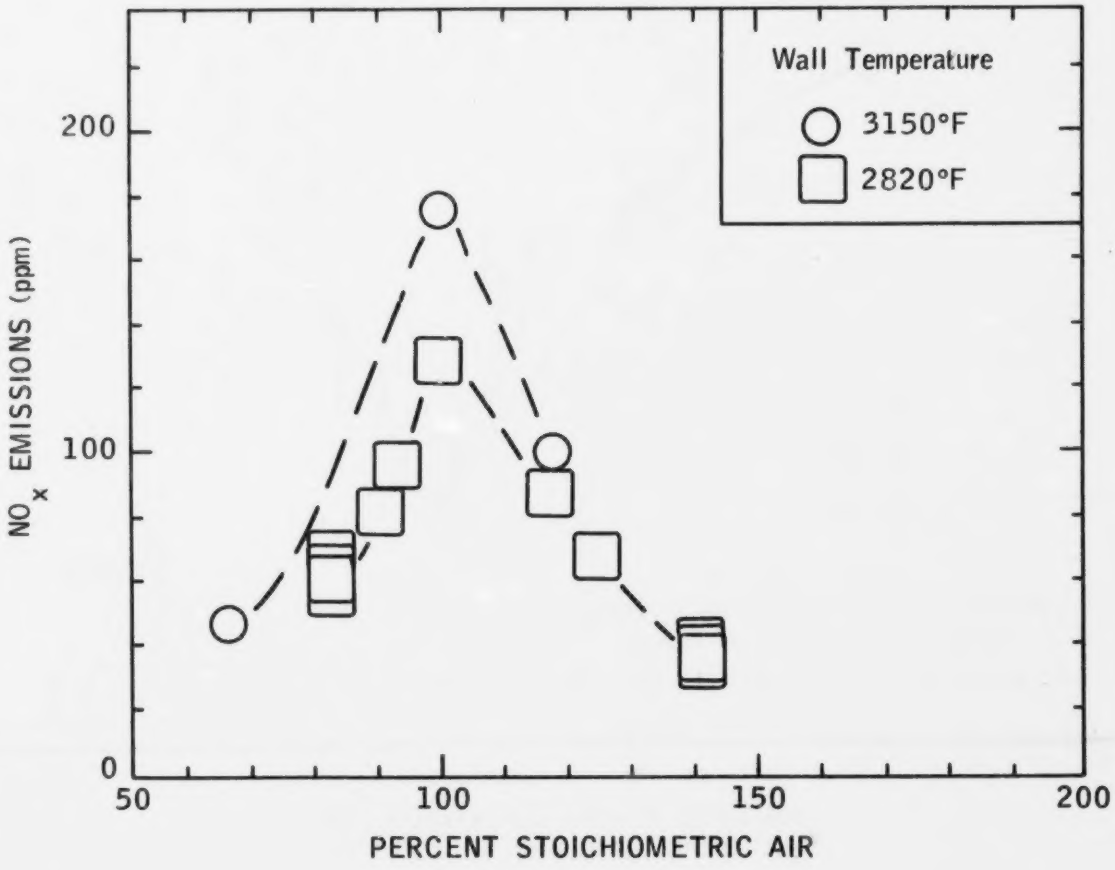


Figure 2-24

EFFECT OF WALL TEMPERATURE ON
NO_x FORMATION IN MULTIBURNER



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3. MATHEMATICAL MODEL OF NO FORMATION IN COMBUSTION PROCESSES

In Phase I of Esso's "Systems Study of Nitrogen Oxide Control Methods for Stationary Sources (3-1) an idealized "first-generation" mathematical model of NO formation in combustion processes was formulated. The description of this model, its scope and uses were presented in detail in reference (3-1), and are briefly summarized in the following section of this report.

Because of the idealized nature of the first-generation mathematical model, (premixed fuel/oxidizer, simplified kinetics restricted to fuel-lean conditions, plug flow without transport effects) it was felt desirable to extend the scope of this model. The flexible mathematical formulation of the first-generation mathematical model permitted the stepwise incorporation of additional kinetics, and the simulation of particle combustion and mixing effects in combustion processes. Thus, the current version of our mathematical model, utilizing as its base the first-generation model, is still oriented toward the simulation of NO formation in large-scale combustion equipment. The objectives of this model formulation are to simulate the directional effects of known combustion modification techniques on NO emissions, and to provide guidance for the development of other potential combustion modification techniques. Further modeling work would be required to allow the use of the model as a quantitative tool for guiding the design of improved combustion equipment.

3.1 Features of the First-Generation NO Model

The formulation of a mathematical model capable of the quantitative description of chemical kinetics, transport effects, and combustion operating and design parameters is too complex to be used directly at present. This is so because major pieces of information are still lacking on the detailed chemistry of NO formation in combustion reactions (particularly under fuel-rich conditions) and the fluid dynamic and heat transport behavior of flames and combustion gases.

Based on the above consideration, in the Phase I stationary NO_x study at Esso (3-1) a model was formulated based on premixed, gaseous hydrocarbon fuel/air combustion. Methane was used to simulate natural gas combustion. The principal features of this model were the following:

(a) One-dimensional, homogeneous gas phase reaction system. Plug flow formulation consisting of series of stirred reactors.

(b) Specified flow velocity, pressure and flow area profiles.

(c) Specified heat transfer options

- heat transfer rate profiles
- heat transfer coefficients and wall temperature profiles
- gas temperature profiles
- quenching rate profiles

(d) Heat generation described by two-step overall kinetics of hydrocarbon oxidation to CO, followed by CO combustion to CO_2.

(e) Simplified, uncoupled Zeldovich chain kinetics used to calculate NO concentrations under fuel lean conditions; O-atoms assumed to be in equilibrium with molecular O_2.

(f) Multiple point injection of fuel, air or flue gases, allowing the simulation of two stage combustion and flue gas recirculation.

The mass and energy conservation equations were solved by an implicit integration scheme using a Newton-Raphson iteration technique. Compared with explicit integeration schemes, the implicit scheme offered the advantages of not being subject to the "ignition problem", since the resulting equations were equivalent to those for stirred reactors, and of being much more stable than explicit integration schemes which may "fall apart" if the integration step is made too large.

This first-generation Esso model was used to predict the rates of NO formation in large gas fired boilers, as a function of excess air, preheat temperature, and rate of quenching of the combustion gases. Because of its premixed mixture, the model predicted peak NO emissions at about five per cent excess air, instead of a monotonic decrease of NO with decreasing excess air as experienced in actual practice with diffusion flames. Below stoichiometric air supply conditions, the model could not be used to predict NO concentrations, as discussed above. However, in spite of its "idealized" nature, the model's predictions of NO emissions from large gas fired boilers were of the right order of magnitude under excess air combustion conditions. Also, the directional effects of flue gas recirculation and two-stage combustion (operating the first stage with stoichiometric air supply) were correctly simulated for NO emission reduction. Air preheat temperature was shown to be important, resulting in sharply increasing NO concentrations with increasing air preheat temperatures. NO formation rates were predicted to decrease with increasing quenching rates, because of the shorter effective residence times at high temperatures. Below about 2300°F, the NO formed in the post-flame gases became frozen in all of our computer simulation cases.

3.2 Extension of the Esso Mathematical Model

The following were the principal objectives of the continuing development of the Esso model of NO formation in combustion processes:

- Incorporate additional kinetics on the chemistry of NO formation and decomposition to allow its use under fuel-rich combustion conditions.
- Extend the model's capability to include the analysis of particle (liquid or solid) combustion.
- Simulate transport effects by mixing fuel-lean and fuel-rich zones in the combustion process.

The major portions of the model development are discussed in this section. Listings of the computer program, along with input forms and typical printouts, are presented in the Appendix.

3.2.1 Additional Kinetics

As discusssed above, the basic mathematical structure of the first-generation model has been retained. The total mass, individual species, and energy conservation equations are solved by an implicit integration scheme using a Newton-Raphson iteration technique. This flexible mathematical formulation yields a one-dimensional plug flow combustor, which comprises a series of specified size stirred reactors.

In this model, the net generation of NO is described by a homogeneous, Zeldovich-type gas phase reaction system (3-2). The thermal chain reaction scheme used for this model, not coupled with combustion kinetics, consists of the following elementary steps:

$$O_2 + M \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2O + M \qquad (3\text{-}1),\ (3\text{-}2)$$

$$O + N_2 \underset{k_4}{\overset{k_3}{\rightleftharpoons}} NO + N \qquad (3\text{-}3),\ (3\text{-}4)$$

$$N + O_2 \underset{k_6}{\overset{k_5}{\rightleftharpoons}} NO + O \qquad (3\text{-}5),\ (3\text{-}6)$$

$$N + OH \underset{k_8}{\overset{k_7}{\rightleftharpoons}} NO + H \qquad (3\text{-}7),\ (3\text{-}8)$$

Steady-state treatment of the above scheme yields the net rate of NO formation:

$$\frac{d(NO)}{dt} = \frac{2\ K_o(O_2)}{k_5(O_2) + k_4(NO) + k_4(OH)_{eq}} \quad k_3k_5(N_2)(O_2)$$

$$+ k_3k_7(N_2)(OH)_{eq} - k_4k_6(NO)^2 - k_4k_8\frac{(NO)^2(H)_{eq}}{\sqrt{K_o(O_2)}} \qquad (3\text{-}9)$$

where $K_o = k_1/k_2 = \frac{(O)^2}{(O_2)}$, and hydrogen atoms and hydroxyl radicals are assumed to be present in equilibrium with other combustion species. Neglecting the contribution of reactions (3-7) and (3-8), which have been shown to be significant only under fuel-rich conditons (3-3,3-4) equation (3-9) reduces to the steady state expression for the Zeldovich chain mechanism of atomic exchange reactions.

The following values of the rate coefficients were used for model calculations:

$k_3 = 1.36 \times 10^{14} e^{-75400/RT}$ cc. mole^{-1} sec^{-1}

$k_4 = 3.1 \times 10^{13} e^{-334/RT}$ cc. mole^{-1} sec^{-1}

$k_5 = 6.43 \times 10^{9} T e^{-6250/RT}$ cc. mole^{-1} sec^{-1}

$k_6 = 1.55 \times 10^{9} T e^{-38640/RT}$ cc. mole^{-1} sec^{-1}

$k_7 = 4.1 \times 10^{13} e^{-800/RT}$ cc. mole^{-1} sec^{-1}

$k_8 = 16.4 \times 10^{13} e^{-48,600/RT}$ cc. mole^{-1} sec^{-1}

where the values of k_3, k_4, k_5 and k_6 were taken from the Leeds evaluation (3-5), while k_7 and k_8 are based on the data of Campbell and Thrush (3-6). For comparison purposed lower values of k_3 and k_4 were also used based on the evaluation of Bortner (3-7):

$k_3 = 6.8 \times 10^{13} e^{-75,000/RT}$ cc. mole^{-1} sec^{-1}

$k_4 = 1.5 \times 10^{13}$ cc. mole^{-1} sec^{-1}

Throughout the calculations, oxygen atoms were assumed to be in equilibrium with molecular O_2, according to reactions (3-1) and (3-2). The equilibrium

$$K_o = \frac{k_1}{k_2} = \frac{(O)^2}{(O_2)} = 25e^{-118,000/RT} \qquad (3\text{-}10)$$

was based on the data of the JANAF Thermochemical Tables (3-8) over the range of temperatures of interest.

As in the first-generation NO model, the present formulation requires the input of specified flow velocity, pressure and flow area profiles in addition to gas temperature profiles or quenching rate profiles. Heat generation is described by two-step overall kinetics of hydrocarbon oxidation to CO, followed by CO oxidation to CO_2. The rate data used in the model for the two-step hydrocarbon oxidation are those determined by Morgan for methane combustion in a jet-mixed reactor under fuel-lean conditions (3-9):

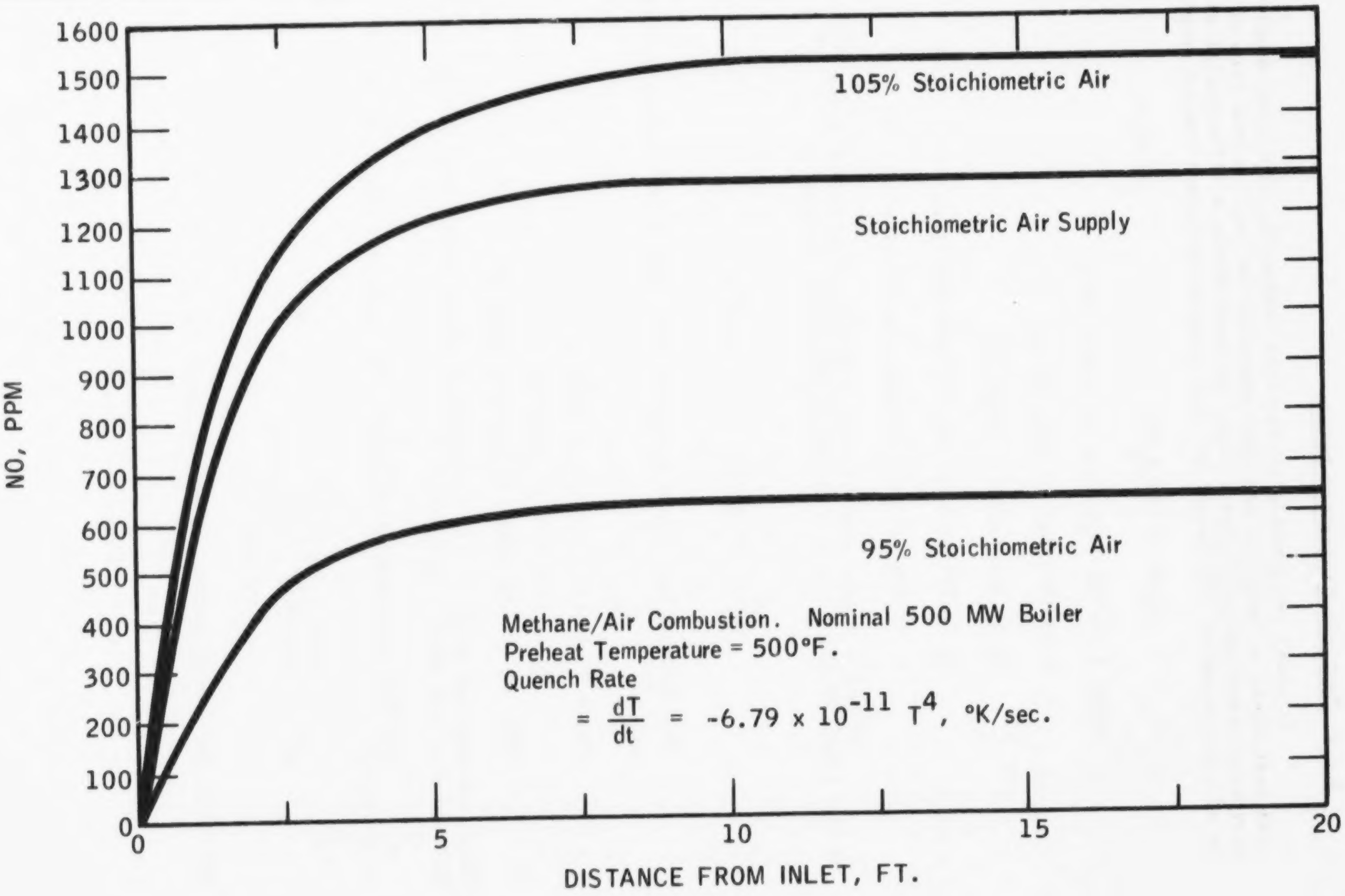
$$\frac{-d(CH_4)}{dt} = 1.8 \times 10^{10} e^{-25,000/RT} (X_{CO})(X_{O2})^{1/2}(X_{H2O})^{1/2}\left(\frac{P}{RT}\right) \qquad (3\text{-}11)$$

where reaction rates are given in g. moles/1./sec., P is the absolute pressure in atmospheres, T is the absolute temperature in °K, and X represents the mole fraction of the species involved in equation (3-11). The use of these overall rate expressions leads to predictions of very rapid fuel burn-out, and consequently, to exhausting the available oxygen. This becomes a significant factor especially under fuel rich or near stoichiometric conditions, and therefore, a constraint is imposed in the model on the O_2 concentration, which is not allowed to decrease below its prevailing equilibrium value.

Typical model predictions of the formation of NO in a natural gas (methane) fired, 500 MW utility boiler as a function of mixture ratio are presented in Figure 3-1. The rate data of reference (3-7) were used in these calculations. In agreement with the trend observed in actual boiler emissions, NO concentration levels increase with increasing air supply over the range of 95% to 105% stoichiometric air. As noted earlier, because of the premixed nature of the model, it predicts peak NO concentrations at about five percent excess air, in contrast with the behavior of diffusion flames which exhibit peak NO conentrations at much higher levels of excess air. The actual levels of "frozen" NO concentrations predicted by our model are on the right order of magnitude, although they tend to be high. This is likely to be due to the idealized (premixed one-dimensional) nature of the model, to the uncertainties in the values of the kinetic rate coefficients, and to the particular quenching rate assigned to these predicitions.

Figure 3 - 1

EFFECT OF MIXTURE RATIO ON NO MODEL PREDICTIONS



3.2.2 Particle Combustion Model

To model the process of particle combustion (fuel oil droplets and coal particles) an analysis was made assuming the fuel in the form of shrinking spherical particles. Thus, by considering a differential element Δx of the combustor, the amount of fuel evaporated from a liquid droplet is:

$$L_o - L = EN_v A_p a\Delta x \qquad (3\text{-}12)$$

where L is the flow rate of liquid fuel

E is the rate of evaporation

N_v is the particle density

A_p is the surface area of the particles

a is the cross-sectional area of flow

Having a weight distribution function of particle sizes f_w^i, at the limit as $\Delta x \longrightarrow 0$, the above expression becomes

$$\frac{dL^i}{dx} = E^i f_w^i A_p^i a \qquad (3\text{-}13)$$

For evaporating liquid droplets, the "shrinking" diameter is given by $D^2 = D_o^2 - Kt$

where D is the diameter at time t

D_o is the initial diameter

and K is the evaporation rate constant

Thus, knowing the density, the quantity of liquid evaporated can be calculated from the above expression.

For the i-th droplet diameter, the fuel particle flow rate $\dot{N}^i$ is given by

$$d\dot{N}^i = \frac{3\,\dot{W}_{fuel}\;{}^{i}_{w}\,dD^i}{\pi\,(D^i)^3\rho}$$

The total fuel vaporization (or gasification rate) is

$$m = \frac{\overset{i}{\Sigma}\,\dot{N}^i\,\rho_\pi\left[(D_o{}^i)^3\right] - (D^i)^3}{6} \qquad (3\text{-}14)$$

The combustion of solid coal particles was analyzed and programmed for the model in a similar manner. In contrast to the burning of liquid sprays where the first step is the relatively slow evaporation of the drops, and the second step is the rapid combustion of vaporized fuel, in coal combustion surface reactions are important. In the present model formulation, it was assumed that a pseudo-gasification step which is mathematically equivalent to the evaporation of liquid drops could be used for coal particles, followed by essentially instantaneous gas phase combustion. Therefore, the evaporation rate becomes and empirical surface burning rate for coal particles, and the modeling equations remain the same.

Model predicitions for the formation of NO in the combustion of fuel oil droplets of uniform size (150μ radius) are presented in Figure 3-2. Again, the computer calculations on which Figure 3-2 is based were carried out for a nominal 500 MW boiler, fired with residual fuel oil having the empirical composition $C_nH_{1.7n}$. The predicted level of NO emisssions shown in Figure 3-2 is clearly much too high for this hypothetical case. Further model development work and testing is required for the assessment of the utility of this approach.

3.2.3 "Macromixing" Model

To simulate the effects of mixing fuel-rich and fuel lean regions in the combustion zone, a "macromixing" analysis was performed and programmed for the model. While not equivalent to a rigorous description of the fluid dynamics of flames, it was felt that based on present knowledge such a macroscopic treatment can provide useful insight into mixing effects on NO formation.

The "macromixing" model, shown schematically in Figure 3-3 as a combination of two parallel-series stirred tank reactor with transport exchange is somewhat similar to the gas turbine model of Hammond and Mellor (3-10). However, instead of using a pair of parallel stirred tank reactors followed by a series of other stirred tank reactors as in the Hammond-Mellor model, the Esso macromixing formulation is comprised of two series of parallel stirred tank reactors, in which transport is allowed at each stage until the concentrations become the identical.

In the macromixing model, one series of reactors represents the fuel-rich region of combustion, while the other one represents the fuel-lean region. Mixing is simulated by allowing transport exchanges to occur at specified rates between each set of parallel reactors.

The number of parallel-series reactors is dependent on the rate of transport exchange between the reactors. Once significant changes cease to exist in the conditions of the two parallel streams (concentrations and temperatures), the parallel-series arrangement is merged into a single train.

In Figure 3-4, a simulation of staged or "off-stoichiometric" firing is presented for a 500MW, gas fired utility boiler using the macromixing model. The model predictions on NO formation in mixing a fuel-rich zone (representing

Figure 3 - 2

MODEL PREDICTION OF NO FORMATION IN FUEL OIL DROPLET COMBUSTION

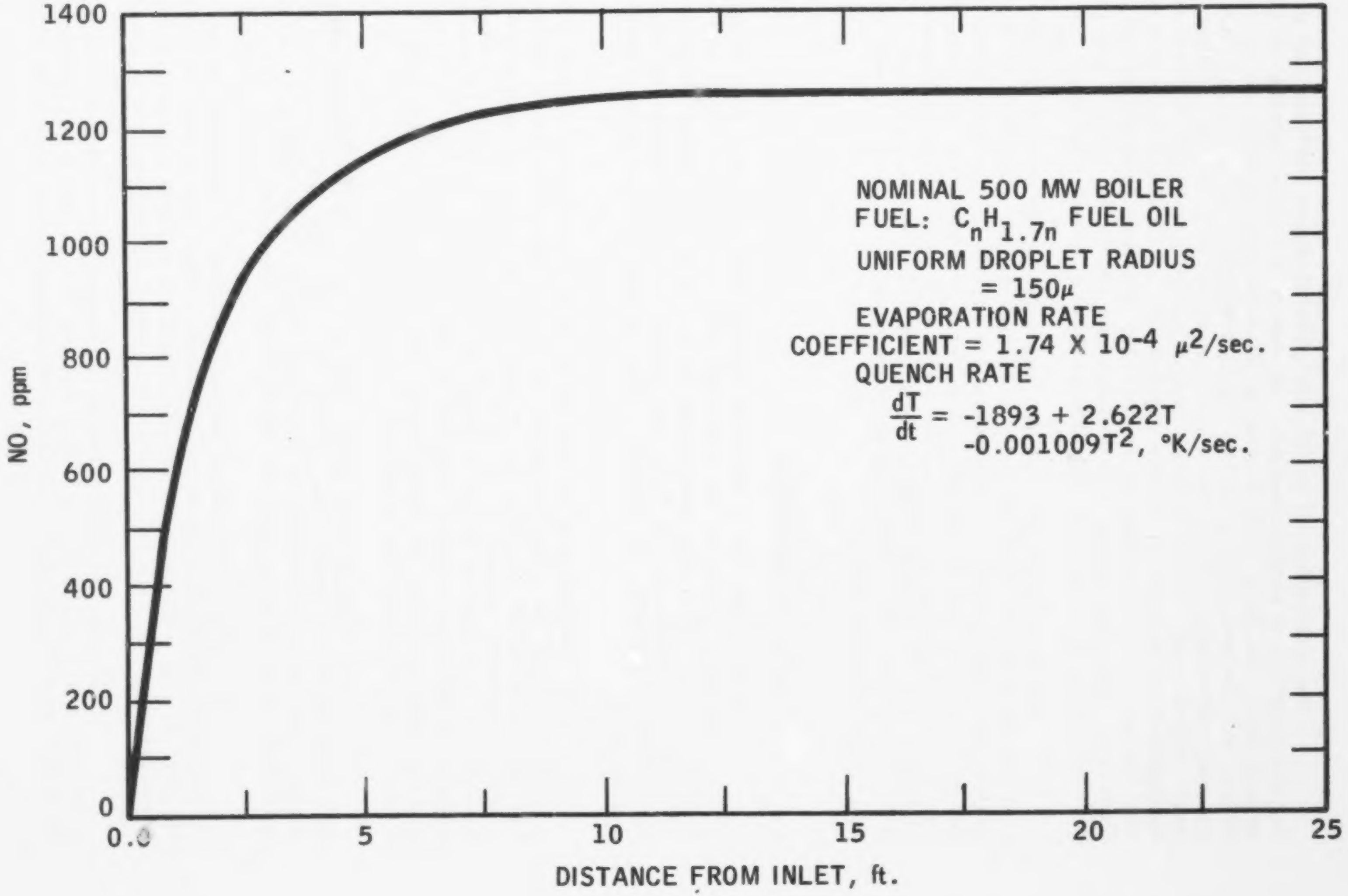


Figure 3 - 3

PARALLEL-SERIES "MACROMIXING" MODEL

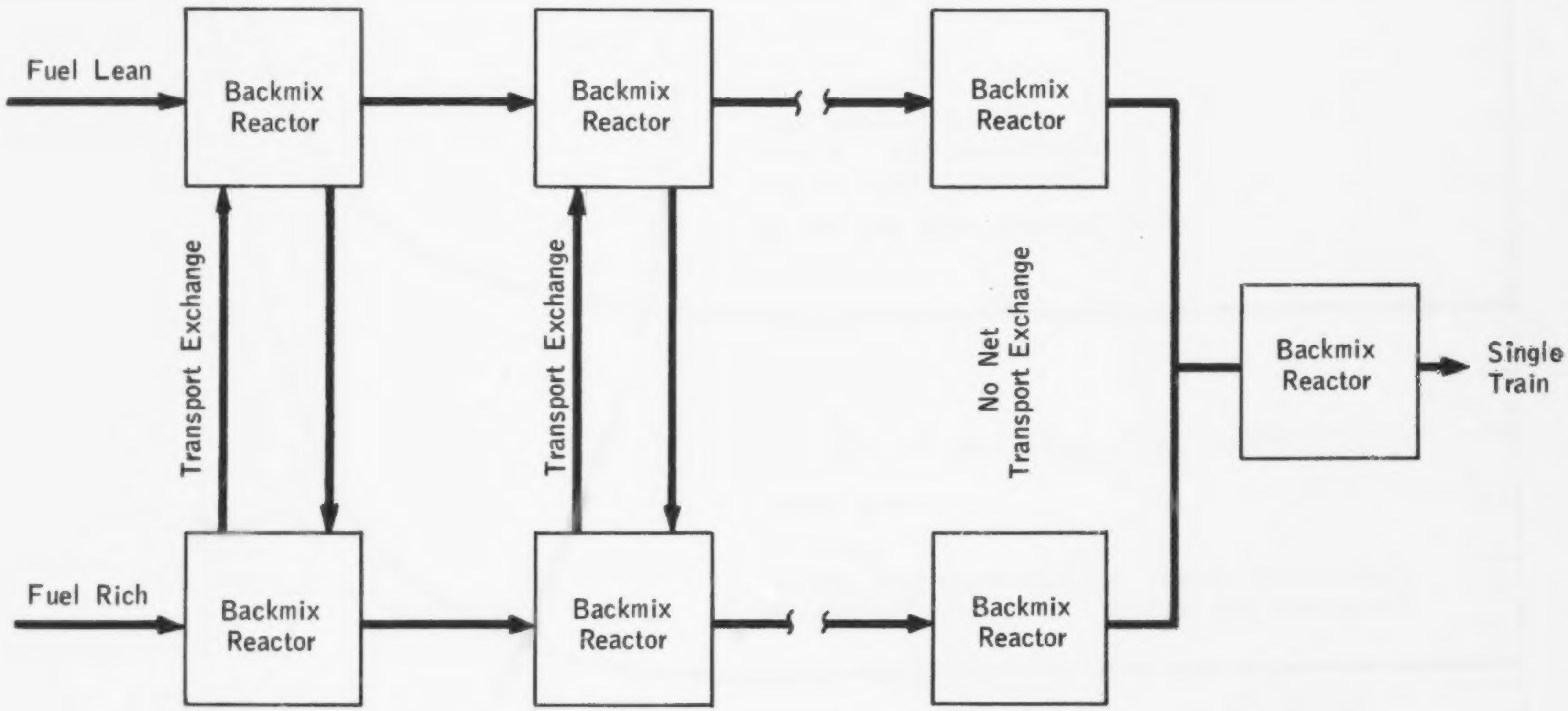
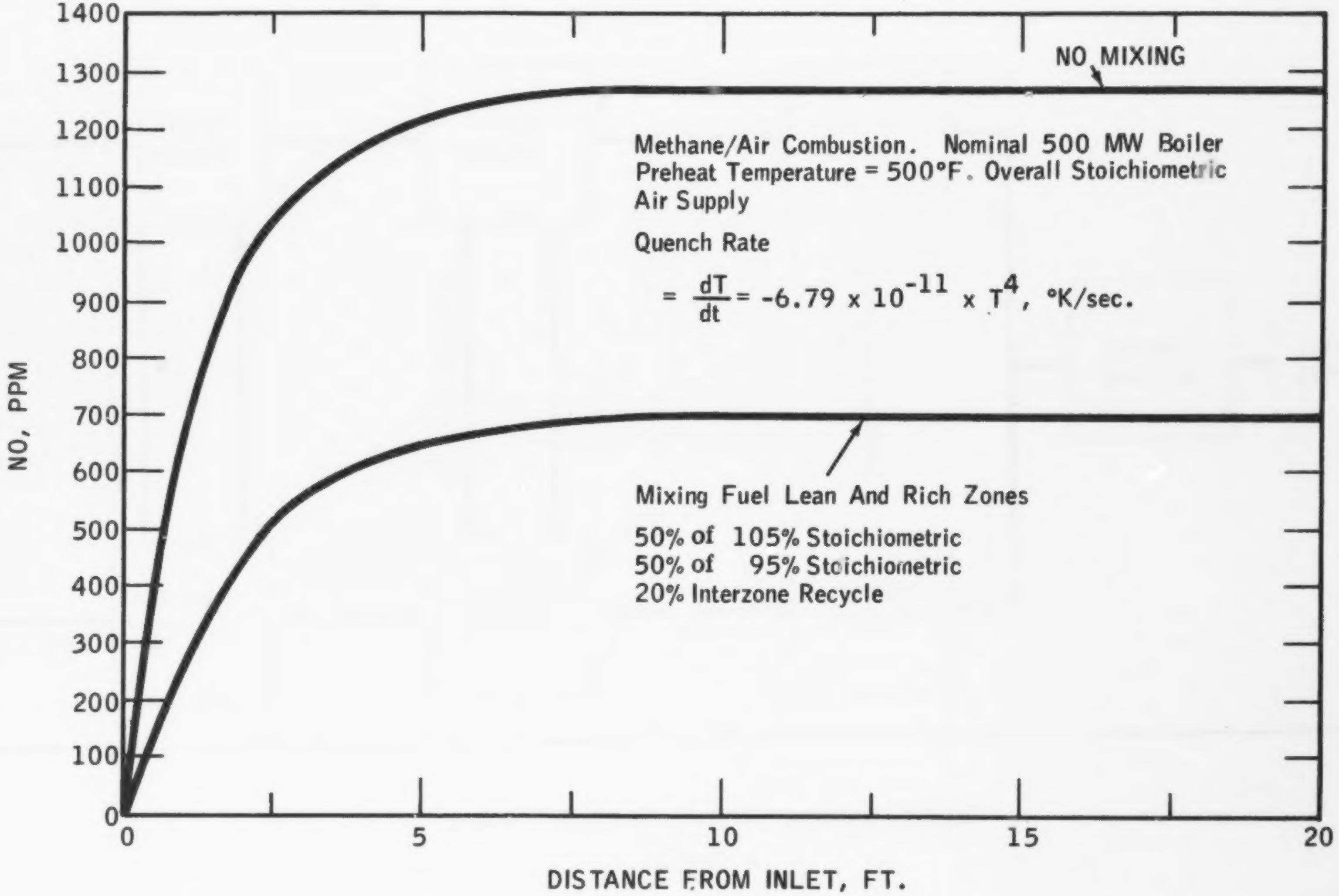

Fuel Lean
Fuel Rich
Backmix Reactor
Backmix Reactor
Backmix Reactor
Backmix Reactor
Backmix Reactor
Backmix Reactor
Backmix Reactor
Transport Exchange
Transport Exchange
No Net Transport Exchange
Single Train

Figure 3 - 4

EFFECT OF MACROMIXING ON NO MODEL PREDICTIONS



50% of the furnace) initially at 95% stoichiometric air with a fuel-lean zone initially at 105% stoichiometric air are compared with model predictions of NO formation corresponding to conditions in the absence of mixing. As shown in Figure 3-4, the macromixing model predicts about a 40% decrease in NO, compared with the no mixing case. This finding is in directional agreement with "off-stoichiometric" or staged firing experience in utility boilers (3-11), (3-12). Thus, the use of this type of approach with detailed parametric variations may lead to a better understanding of the importance of mixing effects on NO formation in combustion processes.

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4. CONCLUSIONS AND RECOMMENDATIONS

from B1

4.1 Conclusions

Basic factors influencing the formation of nitrogen oxides in combustion were investigated experimentally and theoretically in this study. The combustion conditions were selected to be pertinent to stationary sources such as furnaces and boilers with peak temperatures ranging from 2500-3500°F. The following results were obtained:

to B2

(1) NO_x emission profiles were established for a jet-stirred combustor in which the combustion was not limited by mixing. The combustor was used with methane, propane, carbon monoxide, and hydrogen as fuels with air as the oxidizer.

  (a) A strong dependence on mixture ratio was found with peak emissions occurring under slightly fuel-rich conditions. Because of the well-stirred nature of the combustor, with reactants mixing very rapidly with products, there is a measurable oxygen concentration in the reation zone even under fuel-rich conditions.

  (b) As residence time in the reaction zone increased, the temperature in the zone decreased because of heat losses. The effect of increasing residence time and decreasing temperature offset each other resulting in constant emissions at constant preheat in our combustor. Changing preheat altered the emissions. Thus, both residence time and preheat temperature (i.e., combustion temperature) influenced NO_x emissions.

  (c) Peak NO_x emissions for methane/air burning at 3300°F at a nominal residence time of 2 msec at 90% stoichiometric air were found to be 100 ppm; emissions fell off at richer and leaner mixtures, becoming less than 10 ppm below 60% stoichiometric air and above 150% stoichiometric air.

  (d) Results for propane/air and carbon monoxide/air were similar, although with slightly higher NO_x emissions. Hydrogen, even though burning at higher temperatures, exhibited lower NO_x emissions than any of the other fuels used.

(2) NO formation in the jet-stirred combustor (methane/air) exceeded that predicted by the Zeldovich mechanism (based on the "equilibrium oxygen atom" assumption), in some cases by an order of magnitude. However, since the Zeldovich mechanism was developed for use in the post-flame zone, and since the jet-stirred combustor is entirely a flame zone reactor, the disagreement is not entirely unexpected.

(3) Evidence of coupling between combustion kinetics and NO formation kinetics was obtained when methane was added to hydrogen combustion and when CO was added to hydrogen combustion. The resulting emissions were more than a simple additive effect. The results were not inconsistent with the production of "super-equilibrium" oxygen atoms in the combustion zone caused by the presence of methane or carbon monoxide.

(4) Nitrogen bond-type additives were used in methane-air combustion to investigate the effect of N-O, N-H, and N-C bonds in the combustion zone on NO_x emissions. The emissions were similar for the above bond-types when they were added at the same concentrations. Small differences were noted with retention or conversions for $NO > NH_3 > CH_3NH_2 > (CN)_2$. The emissions for the addition of NO_2 were similar to those for NO except that NO_2 exhibited a peak above NO at about 110% stoichiometric air.

(5) Nitrogen bond-type additive conversions to NO_x exhibited a dependence on mixture ratio on the fuel-rich side dropping off to nearly zero at approximately 60% stoichiometric air. Conversions were essentially constant on the fuel lean side out to approximately 150% stoichiometric air, dropping off slightly above 150%. The conversion percentages in the jet-stirred combustor were essentially independent of additive concentration up to about 3000 ppm.

(6) The multiburner (so-called because it can burn gas, oil, or pulverized coal) was designed, constructed, and tested. The formation of NO_x in heated air was found to be linear with residence time. Flow rate of methane/air burning in the combustion zone was found to have a small effect on NO_x emissions. Wall temperature of the combustion zone was found to have an effect on NO_x emissions.

(7) The mathematical model extension has been accomplished. The model now can handle fuel-rich combustion, particle combustion, and macroscopic mixing effects in combustion. Test cases have been run. The model predicts the correct order of magnitude NO_x emissions for boilers. The directional trends for combustion modifications are simulated.

(8) The model predicts much lower NO emissions than found experimentally in the jet-stirred combustor. The model is not formulated with coupled combustion kinetics and NO formation kinetics. Coupled kinetics are needed for calculations related to the jet-stirred combustor.

(9) For boilers emitting more than 300 ppm NO_x emissions coupled chemical kinetics appears to be of lesser importance. However, when attempts are made to reach the range 100-200 ppm or less, coupled kinetics may become more important. For large natural gas boilers operating at high NO_x levels, post-flame NO_x formation appears to dominate; however, fixation of atmospheric nitrogen in the flame zone could become significant at low NO_x levels. For fuels containing nitrogen compounds, techniques to minimize conversion to NO_x may involve a competition between oxidation kinetics and dissociation/recombination kinetics.

4.2 Recommendations for Future Work

The results of this study indicate that under selected combustion conditions significant quantities of NO_x can be formed in the flame zone. There is also good evidence for the coupling between nitrogen oxide formation reactions and combustion reactions. Further study is required to relate the kinetics and mechanisms of pollutant formation reactions and those of other combustion reactions.

Future studies on such coupling effects should include the study of the flame zone and post-flame zone under well-defined conditions. The following variables should be investigated:

- Fuel type
- Flame configuration (premixed, diffusion)
- Fuel/air mixture ratio
- Combustion air preheat
- Rate of heat removal from combustion zone
- Firing rate

The multiburner can be used to study pollutant formation under realistic combustion conditions with controlled heat losses from the flame and post-flame zones. Temperature and species profiles should be determined throughout the combustion zone to characterize the coupling between combustion reactions and pollutant formation. The role of combustion intermediates as well as the stable gas concentrations should be investigated. The combustion of hydrogen, carbon monoxide, methane, and propane, respectively with air should be investigated to determine the coupling of kinetics effects under specific conditions.

The jet-stirred combustor should be used to support and aid interpretation of the experiments performed with the multiburner. The jet-stirred combustor allows the study of combustion under kinetically limited conditions since transport phenomena are not limiting. Comparison of experimental findings with theoretical calculations for a well-determined combustion system such as hydrogen-air should validate the use of the combustor as a kinetic tool. Calculations on a complex combustion system such as hydrocarbon (e.g. methane or propane)-air could then be used to validate combustion mechanisms for the conditions of the jet-stirred combustor. Systems such as carbon monoxide-air could be used as a case of intermediate complexity between the "simple" hydrogen-air system and the "complex" hydrocarbon-air systems.

Kinetics calculations and mathematical modeling play a vital role in the understanding of combustion phenomena. In addition to the kinetics calculations required for interpretation and understanding of the experimental work, further attention should be given to the modeling of combustion processes occurring in large boilers. Further sophistication in the chemical kinetics and fluid mechanics of such a model is desirable, since even simplified models of combustion systems can provide insight into the effect of various combustion parameters on pollutant formation.

Mathematical techniques are currently available to provide extreme sophistication in both chemical kinetics calculations and fluid mechanical representations and it is desirable to incorporate as much sophistication as feasible from the standpoint of (1) our knowledge of the reliability of input parameters for such sophisticated models and (2) the computer technology available to perform such detailed calculations (both from a systems and cost standpoint).

Basic research in both chemical kinetics and fluid mechanics is the foundation upon which understanding of combustion and combustion modeling rests. Without the clear knowledge of appropriate values of the rate coefficients for the significant for a given system, the calculations which lead to a detailed understanding of combustion processes cannot achieve their ultimate potential. Research on the determination of cannot achieve their ultimate potential. Research on the determination of rate constants for crucial reactions is therefore necessary. Furthermore, appropriate fluid mechanic modeling and methods of calculating the required mixing parameters must be coupled to the kinetics calculations for application to the operation of combustion equipment. Detailed heat transfer modeling ultimately must be coupled to the above components of combustion to make the calculations more rigorous.

A research program as described above, with components extending from the basic to the applied, will lead to an understanding of pollutant formation and a detailed understanding of the factors which affect this formation. The ultimate goal of such a research program is the development of control technology applicable to full-scale combustion equipment.

APPENDIX A

EXPERIMENTAL RESULTS JET-STIRRED COMBUSTOR

TABLE A-1

Methane/Air, Effect of Mixture Ratio

Fuel Flow (1/sec)	Air Flow (1/sec.)	Percent Stoichiometric Air	Gas Temperature (°F)	NO_x Emission (ppm)	O_2 Conc. (% Dry)
0.071	0.98	145	2810	7	
0.076	0.98	135	2950	14	
0.081	0.98	127	3110	25	4.6
0.086	0.98	120		44	3.2
0.092	0.98	112		64	2.2
0.092	0.98	112		67	2.6
0.086	0.98	120		43	4.2
0.081	0.98	127	3000	28	
0.076	0.98	135	2850	15	
0.071	0.98	145	2710	8	
0.066	0.98	156	2580	5	
0.071	0.98	145	2835	8	
0.092	0.98	112		55	3.3
0.081	0.98	127	2910	22	
0.086	0.98	120	3000	35	
0.097	0.98	106		70	
0.104	0.98	99		95	
0.140	0.98	74		60	
0.118	0.98	87		100	
0.108	0.98	95		90	
0.083	0.98	124		25	5.5
0.122	0.98	84		90	0.5
0.144	0.98	71		30	0.3
0.092	0.98	112		53	3.5
0.010	0.98	103		68	1.0
0.134	0.98	77		64	0.3
0.071	0.98	145		6	7.1
0.092	0.98	112		44	2.6
0.155	0.98	66		24	3.9

TABLE A-2

Methane/Air, Effect of Residence Time

Fuel Flow (1/sec)	Air Flow (1/sec.)	Percent Stoichiometric Air	Gas Temperature (°F)	NO_x Emission (ppm)
0.092	1.35	154	2810	7
0.102	1.35	139	2950	14
0.112	1.35	127	3190	23
0.122	1.35	116		35
0.144	1.35	98		95
0.190	1.35	75		75
0.197	1.35	72		40
0.208	1.35	68		23
0.058	0.61	110	2910	42
0.074	0.795	113	2950	47
0.092	0.98	112	3110	57
0.108	1.16	113		67
0.060	0.61	107	2950	60
0.081	0.61	79	3030	90
0.110	0.795	76	3030	85
0.131	0.98	79	3140	90
0.098	0.61	65	2910	50
0.124	0.795	67	2950	43
0.177	1.16	69	2925	50
0.112	0.61	57	2800	23
0.049	0.61	131	2790	23
0.063	0.795	133	2800	15
0.079	0.98	130	2950	22
0.094	1.16	130	2990	20
0.043	0.61	149	2350	4
0.056	0.795	149	2470	4
0.066	0.98	156	2580	5
0.082	1.16	149	2700	5
0.077	0.61	83	3110	100
0.098	0.795	85	3110	100
0.118	0.98	87		95
0.081	1.16	150		8
0.140	1.16	87		95
0.056	0.61	114		30
0.068	0.61	94	3110	95
0.068	0.98	151	2500	2
0.089	0.795	94		100
0.108	0.98	95		97
0.073	0.98	141		5

TABLE A-3

Propane/Air Combustion

Fuel Flow (1/sec)	Air Flow (1/sec.)	Percent Stoichiometric Air	Gas Temperature (°F)	NO_x Emission (ppm)
0.0425	0.61	60		49
0.0495	0.61	52		7
0.026	0.61	99	2950	105
0.023	0.61	111	2910	70
0.0195	0.61	131	2800	40
0.0165	0.61	155	2530	8
0.0195	0.61	131	2650	29
0.023	0.61	111	2850	60
0.026	0.61	99	2950	90
0.0295	0.61	87	2950	120
0.036	0.61	71	2990	100
0.0425	0.61	60	2835	50
0.023	0.61	111	2835	50
0.0295	0.61	87	2990	110
0.033	0.61	78	3020	118
0.036	0.61	71	3020	102
0.033	0.61	78	3050	119
0.0425	0.61	60	2835	55
0.0165	0.61	155	2400	6

TABLE A-4

Hydrogen/Air Combustion

Fue[illegible]low ([illegible]ec)	Air Flow (l/sec.)	Percent Stiochiometric Air	NO_x Emission (ppm)
0.127	0.70	232	0
0.155	0.70	190	0
0.182	0.70	162	0
0.210	0.70	140	7
0.545	0.70	54	18
0.450	0.70	65	13
0.390	0.70	75	(25)
0.298	0.70	99	(45)
0.420	0.70	70	20
0.380	0.70	77	(35)
0.327	0.70	90	(60)
0.265	0.70	111	(40)
0.700	0.70	42	25
0.450	0.70	65	15
0.420	0.70	70	20

TABLE A-5

Carbon Monoxide/Air Combustion

Fuel Flow (l/sec)	Air Flow (l/sec.)	Percent Stoichiometric Air	NO_x Emission (ppm)
0.216	0.61	118	80
0.259	0.61	98	97
0.300	0.61	87	120
0.341	0.61	76	110
0.175	0.61	146	20
0.300	0.61	87	118
0.341	0.61	76	80
0.389	0.61	67	65
0.509	0.61	50	30
0.436	0.61	59	50

TABLE A-6

Nitric Oxide Additition

Fuel Flow (1/sec)	Air Flow (1/sec.)	Percent Stoichiometric Air	Equivalent NO Addit. (ppm)	Net NO Increase (ppm)	Gas Temperature (°F)
0.083	0.98	124	100	80	3030
0.083	0.98	124	290	235	3050
0.083	0.98	124	504	450	2925
0.083	0.98	124	100	87	3020
0.071	0.98	145	293	208	
0.092	0.98	112	288	235	
0.112	0.98	92	282	162	
0.089	0.98	116	102	96	
0.081	0.98	127	102	81	
0.081	0.98	127	291	225	
0.081	0.98	127	497	425	
0.083	0.98	124	240	205	3170
0.112	0.98	92	234	200	
0.134	0.98	77	229	130	
0.144	0.98	71	227	135	
0.155	0.98	66	225	95	
0.071	0.98	145	1366	1160	2640
0.092	0.98	112	1340	1180	3155
0.112	0.98	92	1316	1080	
0.134	0.98	77	1291	785	
0.155	0.98	66	1267	430	
0.092	0.98	112	434	400	2800
0.092	0.98	112	1165	1180	2800
0.092	0.98	112	1898	1820	2800
0.150	0.98	69	1804	840	2925
0.150	0.98	69	2774	1240	2865

TABLE A-7

Nitrogen Dioxide Addition

Fuel Flow (l/sec)	Air Flow (l/sec.)	Percent Stoichiometric Air	Equivalent NO Addit. (ppm)	Increase (ppm)	Gas Temperature (°F)
0.083	0.98	124	139	140	
0.083	0.98	124	380	375	
0.083	0.98	124	670	675	
0.830	0.98	124	720	725	
0.071	0.89	145	300	275	2580
0.092	0.98	112	298	310	3155
0.112	0.98	92	292	280	
0.134	0.98	77	286	210	
0.155	0.98	66	280	112	2880
0.083	0.98	124	300	300	3000

TABLE A-8

Ammonia Addition

Fuel Flow (l/sec)	Air Flow (l/sec.)	Percent Stoichiometric Air	Equivalent NO Addit. (ppm)	Net NO Increase (ppm)	Gas Temperature (°F)
0.085	0.98	121	100	75	3110
0.085	0.98	121	211	178	3080
0.085	0.98	121	504	455	3000
0.085	0.98	121	100	85	3080
0.083	0.98	124	504	415	3050
0.083	0.98	124	504	395	3020
0.071	0.98	145	1367	918	2650
0.092	0.98	112	1341	850	3110
0.112	0.98	92	1316	724	
0.134	0.98	77	1291	600	
0.155	0.98	66	1268	165	
0.092	0.98	112	495	340	3110
0.092	0.98	112	1045	840	3110
0.092	0.98	112	1633	1220	3110
0.092	0.98	112	2195	1625	3125
0.092	0.98	112	1924	1415	3125
0.092	0.98	112	2195	1675	3110
0.092	0.98	112	2775	1870	3185
0.071	0.98	145	1366	920	2790
0.092	0.98	112	1341	965	
0.112	0.98	92	1317	730	
0.134	0.98	77	1291	430	
0.155	0.98	66	1267	115	

TABLE A-9

Cyanogen Addition

Fuel Flow (l/sec)	Air Flow (l/sec.)	Percent Stoichiometric Air	Equivalent NO Addit. (ppm)	Net NO Increase (ppm)	Gas Temperature (°F)
0.083	0.98	124	200	140	
0.083	0.98	124	650	412	
0.083	0.98	124	1008	700	
0.083	0.98	124	421	310	
0.083	0.98	124	200	130	
0.071	0.98	145	547	272	2400
0.092	0.98	112	536	350	3110
0.112	0.98	92	527	300	
0.134	0.98	77	516	220	
0.155	0.98	66	507	8	2950
0.144	0.98	71	512	80	3110
0.071	0.98	145	2733	1655	2640
0.092	0.98	112	2681	1780	3110
0.112	0.98	92	2633	1525	
0.134	0.98	77	2582	1010	
0.155	0.98	66	2535	230	
0.092	0.98	112	1000	725	2990
0.092	0.98	112	2089	1330	3000
0.092	0.98	112	3267	1900	3110
0.092	0.98	112	4360	2360	3050

TABLE A-10

Methylamine Addition

Fuel Flow (1/sec)	Air Flow (1/sec.)	Percent Stoichiometric Air	Equivalent NO Addit. (ppm)	Net NO Increase (ppm)	Gas Temperature (°F)
0.071	0.98	145	547	380	2470
0.092	0.98	112	536	390	2910
0.112	0.98	92	527	345	2925
0.134	0.98	77	517	360	2950
0.144	0.98	71	512	175	2830
0.155	0.98	66	507	0	2710
0.092	0.98	112	200	150	2950
0.092	0.98	112	769	665	2940
0.092	0.98	112	1212	1010	2950
0.092	0.98	112	536	410	2950

APPENDIX B

Compressed Gas Compositions

The methane was Matheson Technical Grade with a minimum purity of 98.0%. A typical analysis from Matheson states the following components:

Methane (Technical Grade)

Methane	99.2
Ethane	3100 ppm
Nitrogen	4460 ppm
Carbon Dioxide	350 ppm
Higher alkanes	200 ppm

The hydrogen was Linde C.P. grade with 99.95 minimum purity and a typical water content of 11 ppm.

The carbon monoxide was Matheson C.P. grade, 99.5% minimum purity with the following typical analysis of impurities:

Carbon Monoxide (C.P. Grade)

Carbon dioxide	50 ppm
Oxygen	600 ppm
Nitrogen	1500 ppm
Water	8 ppm
Hydrocarbon (as methane)	40 ppm

The propane was Matheson C.P. grade, 99.0% minimum purity with the following typical analysis of impurities:

Propane (C.P. Grade)

Ethane	500 ppm
Isobutane	5000 ppm
Propylene	500 ppm

The air used was Baker Dry Grade, manufactured by mixing nitrogen and oxygen, with the following typical analysis:

Air (Dry Grade)

Nitrogen	79.0%
Oxygen	21.0%
Argon	450 ppm
Hydrocarbon	3 ppm
Water	3 ppm
Carbon Dioxide	1 ppm

APPENDIX C

PRELIMINARY DATA - MULTIBURNER

TABLE C-1

NO_x FORMATION FROM AIR MULTIBURNER WALL TEMPERATURE 3150°F

Air Flow Rate (SCFM)	Distance from Injection Point (inches)	NO_x (ppm)
2.06	15	55
1.37	15	68
0.685	15	185
3.43	15	33
2.74	15	42
0.685	13	170
0.685	19	226
0.685	15	180
0.685	15	172

TABLE C-2

NO_x EMISSIONS METHANE/AIR COMBUSTION

Fuel Flow Rate (SCFM)	Air Flow Rate (SCFM)	Per Cent Stoichiometric Air	Wall Temperature (°F)	Distance from Injection Point (inches)	NO_x (ppm)
0.430	3.90	95	2820	15	95
0.430	3.43	83	2820	15	65
0.430	3.77	92	2820	15	80
0.430	4.11	100	2820	15	115
0.430	4.80	117	2820	15	85
0.430	5.14	125	2820	15	65
0.430	5.82	142	2820	15	35
0.430	5.82	142	2820	15	30
0.430	6.85	167	2820	15	20
0.430	3.43	83	2820	15	70
0.430	3.43	83	2820	15	60
0.215	1.37	67	3150	15	60
0.215	2.06	100	3150	15	175
0.215	2.74	133	3150	15	75
0.215	2.74	133	3150	15	90
0.215	3.43	167	3150	15	45
0.215	2.06	100	3150	15	185
0.430	2.74	67	3150	15	45
0.430	4.11	100	3150	15	175
0.430	4.80	117	3150	15	100
0.645	4.80	78	3150	15	78
0.645	5.48	89	3150	15	89
0.645	6.85	111	3150	15	111
0.645	6.17	100	3150	15	100
0.645	6.03	98	3150	15	98
0.645	5.89	96	3150	15	96
0.645	6.17	100	3150	15	100
0.645	6.30	102	3150	15	102
0.645	6.51	106	3150	15	106

APPENDIX D

In this section the computer program listing, the input forms and a sample calculation output for the NO model developed in this study are presented.

D.1 Macromixing Analysis

D.1.1 Input Forms for Macromixing Analysis

CARD 0 Title Card for Macromixing Analysis

COLUMN

1-10

11-20

21-30

31-40

41-50

51-60

61-80

CARD 1 OPTION CODES FOR MACROMIXING ANALYSIS

COLUMN						
1-5						IS WALL TEMPERATURE PROFILE TO BE SPECIFIED?*
6-10						IS GAS TEMPERATURE PROFILE TO BE SPECIFIED ? (* *)
11-15						IS HEAT FLUX PROFILE TO BE SPECIFIED ? (*)
16-20						NUMBER OF SECONDARY INJECTION POINTS (MAX OF 20
21-25	☒	☒	☒	☒	☒	LEAVE BLANK
26-30						MIXING ? * * *
31-35						
36-40						
41-45						
46-50						
51-55						
56-60						
61-65						
66-70						

* { 1 = YES, BY USER
0 = NO,

** { 0 = NO
1 = YES, BY USER
2 = YES, FROM QUENCH RATE CALCULATIONS

*** { 1 = YES
0 = NO

NOTE: ALL ITEMS ON THIS CARD MUST BE RIGHT-JUSTIFIED.

ONE, AND ONLY ONE, OF THE FIRST 3 SPECIFICATION OPTIONS MAY BE EXERCISED, i.e., ONLY ONE YES RESPONSE ON FIRST 3 OPTIONS

CARD 2 STOCHIOMETRIC COEFFICIENT FOR $a(FUEL) + b(O_2) \rightarrow c(CO) + d(H_2O)$

COLUMN		
1-10	.	FUEL COEFFICIENT, a = 1
11-20	.	O_2 " , b
21-30	.	CO " , c
31-40	.	H_2O " , d
41-50		
51-60		
61-70		

CARD 3.1 PHYSICAL CONDITIONS OF FUEL-RICH INLET GAS MIXTURE

COLUMN		
1-10	.	FLOW RATE (G-MOLES/SECOND)
11-20	.	TEMPERATURE (°K)
21-30	.	PRESSURE (PSIA)
31-40		
41-50		
51-60		
61-70		

CARD 3.2 PHYSICAL CONDITIONS OF FUEL-LEAN INLET GAS MIXTURE

COLUMN		
1-10	.	FLOW RATE (G-MOLES/SECOND)
11-20	.	TEMPERATURE (°K)
21-30	.	PRESSURE (PSIA)
31-40		
41-50		
51-60		
61-70		

NOTES:

CARD 4.1 INLET GAS COMPOSITION OF FUEL RICH STREAM

COLUMN		
1-10		MOLE FRACTION OF O_2
11-20		" CO_2
21-30		" FUEL
31-40		" CO
41-50		" H_2O
51-60		" N_2
61-70		" NO

CARD 4.2 INLET GAS COMPOSITION OF FUEL LEAN STREAM

COLUMN		
1-10		MOLE FRACTION OF O_2
11-20		" CO_2
21-30		" FUEL
31-40		" CO
41-50		" H_2O
51-60		" N_2
61-70		" NO

CARD 5 CONDITION AND LOCATION OF SECONDARY INJECTION GAS**

COLUMN		
1-10		FLOW RATE (G-MOLES/SEC)
11-20		TEMPERATURE (OK)
21-30		INJECTION POINT (FEET FROM INLET)*
31-40		
41-50		
51-60		
61-70		

NOTES:

* IF AN INJECTION POINT IS ENCOUNTERED WHILE MIXING, MIXING CALCULATIONS WILL STOP. THE PROGRAM ASSUMES THAT AT THE INJECTION POINT ALL GASES ARE WELL MIXED.

** IF NO INJECTION IS USED DO NOT SUBMIT THIS CARD

CARD 6 INJECTION GAS COMPOSITION *

COLUMN		
1-10		MOLE FRACTION OF O_2
11-20		" CO_2
21-30		" FUEL
31-40		" CO ??
41-50		" H_2O
51-60		" N_2
61-70		" NO

* A MAXIMUM OF 20 INJECTION POINTS MAY BE USED. IF NO INJECTION POINTS ARE USED DO NOT SUBMIT CARDS 5 AND 6. INJECTION POINTS MUST BE SUBMITTED IN ORDER OF INCREASING DISTANCE FROM INLET. USE ADDITIONAL CARDS AS NEEDED FOR MORE INJECTION POINTS.

CARD 7 KINETIC RATE CONSTANTS FOR $a(\text{FUEL}) + b(O_2) \rightarrow c(CO) + d(H_2$

COLUMN		
1-10		FREQUENCY FACTOR, A (*)
11-20		ACTIVATION ENERGY, E (CALORIES)
21-30		O_2 EXPONENT, α
31-40		FUEL " , β
41-50		H_2O " , γ
51-60		
61-70		

THE KINETIC RATE EXPRESSION IS -

$$\mathcal{R} = A\, e^{-\frac{E}{RT}} (O_2)^{\alpha} (\text{FUEL})^{\beta} (H_2O)^{\gamma} \quad \text{g-moles/liter-sec};$$

WITH (O_2), (FUEL) AND (H_2O) IN UNITS OF g-MOLES/LITER AND T IN °K.

(*) THIS ITEM MAY BE EXPRESSED AS AN EXPONENTIAL NUMBER, 0.XXXXE±

CARD 8 KINETIC RATE CONSTANTS FOR $CO + \frac{1}{2} O_2 \longrightarrow CO_2$

COLUMN		
1-10		FREQUENCY FACTOR, A (*)
11-20		ACTIVATION ENERGY, E (CALORIES)
21-30		O_2 EXPONENT, α
31-40		CO " , β
41-50		H_2O " , γ
51-60		
61-70		

THE KINETIC RATE EXPRESSION IS -

$$\mathcal{R} = A\, e^{-\frac{E}{RT}} (O_2)^{\alpha} (CO)^{\beta} (H_2O)^{\gamma} \quad \text{g-moles/liter-sec};$$

WITH (O_2), (CO) AND (H_2O) IN UNITS OF g-MOLES/LITER AND T IN °K.

CARD 9 HEAT TRANSFER CONSTANTS

COLUMN		
1-10	•	CONSTANT COEFFICIENT, A
11-20	•	CONVECTION ", B
21-30	•	RADIATION ", C
31-40		
41-50		
51-60		
61-70		

THE HEAT FLUX TO THE WALL IS EXPRESSED AS -

$$q\,(\text{KCAL.}/\text{FT}^2\text{-SEC}) = A + B(T-T_w) + C(T^4-T_w^4),$$

WHERE T AND T_w ARE THE GAS AND WALL TEMPERATURES (°

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THIS CARD IS TO BE SUBMITTED ONLY IF THE WALL TEMPERATURE SPECIFICATION OPTION HAS BEEN EXERCISED ON CARD 1 (A "1" IN COLUMN 5).

CARD 9.5 QUENCH RATE CONSTANTS

COLUMN		
1-10	.	FIRST COEFFICIENT, A
11-20	.	SECOND " , B
21-30	.	THIRD " , C
31-40	.	FORM OF QUENCH RATE (*)
41-50		
51-60		
61-70		

$$(*)\begin{cases} 0.0 = \text{QUADRATIC FORM} \\ 1.0 = \text{EXPONENTIAL FORM} \end{cases}$$

QUADRATIC FORM : $A + BT + CT^2$

EXPONENTIAL FORM : $(A + BT)\, e^{C/T}$

(T IN °K
QUENCH RATE IN °K/SEC)

THIS CARD IS TO BE SUBMITTED ONLY IF THE GAS TEMPERATURE IS TO BE COMPUTED FROM A QUENCH RATE (A "2" IN COLUMN 10 ON CARD 1).

CARD 10 COMBUSTOR PROFILES

COLUMN			
1-10		DISTANCE FROM INLET (FEET)	
11-20		CROSS-SECTIONAL AREA (FT²)	
21-30		PERIMETER (FEET)	
31-40		WALL TEMPERATURE (°K)	(**)
41-50		GAS TEMPERATURE (°K)	
51-60		HEAT FLUX (KCAL/FT²-SEC)	
80		(*)	

CARD 10 COMBUSTOR PROF.LES

COLUMN			
1-10		DISTANCE FROM INLET (FEET)	
11-20		CROSS-SECTIONAL AREA (FT.²)	
21-30		PERIMETER (FEET)	
31-40		WALL TEMPERATURE (°K)	(**)
41-50		GAS TEMPERATURE (°K)	
51-60		HEAT FLUX (KCAL/FT²-SEC)	
80		(*)	

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(*) ENTER A "1" IN COLUMN 80 IF THIS IS THE FINAL PROFILE CARD

(**) ENTER VALUES FOR THE ITEM CORRESPONDING TO THE SPECIFICATION CHOSEN ON CARD 1.

AT LEAST TWO CARDS, ONE FOR THE INLET AND ONE FOR THE OUTLET, MUST ALWAYS BE SUBMITTED (MAXIMUM OF 100 CARDS).

USE ADDITIONAL CARDS AS NEEDED FOR MORE PROFILES.

PROFILE CARDS MUST BE SUBMITTED IN ORDER OF INCREASING DISTANCE FROM INLET.

CARD 11 COMBUSTOR LENGTH AND PRINTOUT INTERVAL

COLUMN		
1-10	.	REACTOR LENGTH (FEET)
11-20	.	PRINTOUT INTERVAL (FEET) (*)
21-30	.	INTEGRATION INTERVAL (FEET) (**)
31-40		
41-50		
51-60		
61-70		

(*) A NUMBER, N, ENTERED HERE WILL CAUSE RESULTS TO BE PRINTED OUT EVERY N FEET ALONG THE COMBUSTOR. THIS NUMBER SHOULD BE AT LEAST AS LARGE AS THE INTEGRATION INTERVAL

(**) IF LEFT BLANK, THE INTEGRATION INTERVAL WILL BE ASSUMED TO BE $1/128^{TH}$ OF THE LENGTH OF A FLAME SEGMENT.

CARD 12 HEAT OF REACTION @ 298 °K

COLUMN		
1-10	.	HEAT OF REACTION (KCAL) FOR REACTION ON CARD 7
11-20	.	HEAT OF REACTION (KCAL) FOR REACTION ON CARD 8
21-30		
31-40		
41-50		
51-60		
61-70		

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CONVENTION: EXOTHERMIC HEAT OF REACTION MUST BE ENTERED AS A NEGATIVE NUMBER.

CARD 13 HEAT CAPACITY DATA FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN					
1-4					NUMBER OF HEAT CAPACITY DATA POINTS, FOR FUEL (*) (298°K ≤ T ≤ 1200°K
5-8					
9-12					
13-16					
17-20					
21-24					
25-28					
29-32					
33-36					
37-40					
41-44					
45-48					
49-52					
53-56					
57-60					
61-64					
65-68					
69-72					

NOTES:

AT LEAST 6 DATA POINTS, INCLUDING VALUES AT 298°K AND 1200°K, MUST BE SUBMITTED. IT IS RECOMMENDED THAT AT LEAST 10 POINTS BE USED (MAXIMUM OF 20).

(*) THIS NUMBER MUST BE RIGHT-JUSTIFIED.

CARD 14 HEAT CAPACITY DATA POINTS FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN

5-14 TEMPERATURE (°K)

15-24 HEAT CAPACITY OF FUEL (CAL/g-MOLE·°K)

CARD 14 HEAT CAPACITY DATA POINTS FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN

5-14 TEMPERATURE (°K)

15-24 HEAT CAPACITY OF FUEL (CAL/g-MOLE-°K)

CARD 14 HEAT CAPACITY DATA POINTS FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN

5-14 TEMPERATURE (°K)

15-24 HEAT CAPACITY OF FUEL (CAL/g-MOLE-°K)

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NOTES:

AT LEAST SIX DATA CARDS MUST BE SUBMITTED, INCLUDING VALUES AT 298°K AND 1200°K. DATA CARDS MUST BE SUBMITTED IN ORDER OF INCREASING TEMPERATURES.

USE ADDITIONAL CARDS AS NEEDED FOR MORE DATA POINTS.

CARD 15 HEAT CAPACITY DATA FOR FUEL (T > 1200°K)

COLUMN					
1-4					NUMBER OF HEAT CAPACITY DATA POINTS FOR FUEL (*) (T > 1200°K)
5-8					
9-12					
13-16					
17-20					
21-24					
25-28					
29-32					
33-36					
37-40					
41-44					
45-48					
49-52					
53-56					
57-60					
61-64					
65-68					
69-72					

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NOTES:

AT LEAST 6 DATA POINTS MUST BE SUBMITTED. IT IS RECOMMENDED THAT AT LEAST 10 POINTS BE USED (MAXIMUM OF VALUES ABOVE 3000°K ARE USUALLY NOT NEEDED.

(*) THIS NUMBER MUST BE RIGHT-JUSTIFIED.

CARD 16 HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200 °K)

COLUMN

5-14 TEMPERATURE (°K)

15-24 HEAT CAPACITY OF FUEL (CAL/g-MOLE - °K)

CARD 16 HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200 °K)

COLUMN

5-14 TEMPERATURE (°K)

15-24 HEAT CAPACITY OF FUEL (CAL/g-MOLE · °K)

CARD 16 HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200 °K)

COLUMN

5-14 TEMPERATURE (°K)

15-24 HEAT CAPACITY OF FUEL (CAL/g-MOLE · °K)

NOTES:

AT LEAST SIX DATA CARDS MUST BE SUBMITTED FOR VALUES ABOVE 1200 °K. DATA CARDS MUST BE SUBMITTED IN ORDER OF INCREASING TEMPERATURES.

USE ADDITIONAL CARDS AS NEEDED FOR MORE DATA POINTS.

CARD 17.1 OXYGEN EQUILIBRIUM RESTRICTIONS FOR FUEL RICH STREAM

COLUMN	
1-10	
11-20	MOLE FRACTION OF O_2 *
21-30	
31-40	
41-50	
51-60	
61-70	

CARD 17.2 OXYGEN EQUILIBRIUM RESTRICTIONS FOR FUEL LEAN STREAM **

COLUMN	
1-10	
11-20	MOLE FRACTION OF O_2 *
21-30	
31-40	
41-50	
51-60	
61-70	

CARD 18 MIXING PARAMETERS

COLUMN	
1-10	
11-20	FRACTION OF TOTAL FUEL SUPPLIED BY FUEL LEAN STR
21-30	FRACTION OF FUEL LEAN STREAM RECYCLED
31-40	FRACTION OF FUEL RICH STREAM RECYCLED
41-50	
51-60	
61-70	

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NOTES:

* IF VALUES ARE NOT KNOWN SUPPLY BLANK CARD

** FOR MIXING OPTION, CARD 17.2 SHOULD ALWAYS BE BLANK

D.1.2 Computer Listing for Macromixing Analysis

```
FORTRAN IV G LEVEL  20                  MAIN                                                    PAGE 0001
0001                DIMENSION DABINV(2),YO(2),Y(2),YOLD(2),GAMBIV(4,2),B(2,2),XZO(4)
0002                DIMENSION GAMMA(4,2),BINV(2,2) ,YO(2),XZOLD(4)
0003                DIMENSION DELALP(2),C?COEF(6,10),                DGIDY(2),DXZDY(4,2)
0004                DIMENSION DCOF(2,14)
0005                DIMENSICN R(2),DRDY(2,2),DRDXZ(2,4),DRDT(2),CP(6),DCPDT(6)
0006                DIMENSION DGCPDY(2),DELH(2),DHDT(2),LMINV(3),MMINV(3),XZ(4)
0007                DIMENSION AJACOE(3,3),FUN(3)
0008                DIMENSICN XPOINT(10 ),AREA(10 ),PERIM(1D ),TWALL(10)
0009                DIMENSIGN QSPEC(10)
0010                DIMENSION TSPEC(10 ),KODE(4)
0011                DIMENSION HTC(3),     RCON(10)
0012                DIMENSION TX(20),CPY(20),C(4),FO(4),F(20,4),A(4,4)
0013                DIMENSION XINJ(20),GINJ(20),TINJ(20),YINJ(2,20),XZINJ(4,20)
0014                DIMENSION YNOINJ(20)
0015                DIMENSION Y2(2),XZ2(4),CPAVG(6)
0016                DIMENSION QNCHRT(3), TCOMBI(20)
0017                DIMENSIGN ICODE(6)
0018                CCMMON/BB/TIME
0019                COMMON/EF/TEST1,KINJEC,KPASSS
0020                CCMMON / FLOOD/ MACRO1
0021                CCMMON/INJECT/XFIN1
0022                DATA CPCOEF/   7.316 ,     4.102,       0.0,   7.705,     8.613,
                  1     7.681, -4.383 ,    22.07 ,      0.0,  -5.617,    -2.632,
                  2    -5.146,  15.23  ,  -24.55 ,      0.0,  13.32 ,     9.036,
                  3     11.42 , -14.26  ,   15.47 ,     0.0, -10.22 ,    -6.405,
                  4    -8.253,   4.429 ,   -4.1  ,      0.0,   2.744,     1.688,
                  5     2.108,  16.67  ,   15.56 ,      0.0,   9.867,    22.94 ,
                  6    10.01 , -24.12  ,   -4.295,      0.0,  -5.465,   -63.02 ,
                  7    -6.693,  49.93  ,    4.718,      0.0,  11.86 ,   154.3  ,
                  8    15.06 , -50.14  ,   -5.741,      0.0, -14.76 ,  -181.7  ,
                  9   -18.80 ,  19.29  ,    2.321,      0.0,   6.559,    78.85 ,
                  A     8.405/
              C
              C
              C**************************************************
              C*    MACROMIXING ANALYSIS OF LEAN-RICH ZONES      *
              C**************************************************
              C
              C
0023                CALL RELOC
0024             40 CONTINUE
0025                IBOMB=0
0026                MACRO1=0
0027                NOPT = 4
0028                NIND = 2
0029                NDEP = 4
0030                NDIM = 3
0031                NCCMP = 6
0032                SS=0.
0033                TIME=0.
0034                KPASSS=0
0035                KINJEC=C
0036                NT=J
```

```
 0037             CALL       ADATA(NIND,NDEP,NCOMP,B,GAMMA,YO,XZO,CPCOEF,DCOF,YNOO,
                 1                  CP,DCPDT,DELH,DHDT,RCON,HTC,XPOINT,AREA,PERIM,
                 2                  TWALL,TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
                 3                  PINT,XINJ,GINJ,TINJ,YINJ,XZINJ,YNOINJ,
                 4                  NOPT,TX,CPY,C,FO,F,A,QNCHRT,QNCHTP,TCOMB,TCOMBI,
                 5                  NSPRAY,ICODE,TB,MACRO)
 0038             TEST1=3.*DELTAX
 0039             C1=-GAMMA(1,1)
 0040             C2=-B(1,1)
 0041             C1= -GAMMA(2,2)
 0042             C2= -B(1,2)
            C        FORM THE ARRAY DELALP WHOSE J'TH ELEMENT CONTAINS THE NET
            C        CHANGE IN MOLES FOR THE J'TH REACTION.
 0043             DO 1 JJ= 1,NIND
 0044             DELALP(JJ)= 0.
 0045             DO 2 II = 1,NIND
 0046           2 DELALP(JJ) = DELALP(JJ)+ B(II,JJ)
 0047             DO 1 II = 1,NDEP
 0048           1 DELALP(JJ) = DELALP(JJ)+GAMMA(II,JJ)
            C        CALCULATE THE INVERSE OF THE 'INDEPENDENT' STOICHIOMETRIC
            C        MATRIX.
 0049             CALL BINVER(NIND,B,BINV)
            C     PREMULTIPLY THE INVERSE OF B BY GAMMA, THE 'DEPENDENT'
            C     STOICHIOMETRIC MATRIX.
 0050             CALL MPRD(GAMMA,BINV,GAMBIV,NDEP,NIND,0,0,NIND)
            C     PRIMULTIPLY THE INVERSE  OF B BY DELALP
 0051             DO 3 JJ = 1,NIND
 0052             DABINV(JJ) = 0.
 0053             DO 3 II = 1,NIND
 0054           3 DABINV(JJ)=DABINV(JJ) + DELALP(II)*BINV(II,JJ)
            C
            C          FOR LIQUID OR SOLID FUELS XZO(1) IS READ IN AS ZERO.
            C          THEREFORE, THE COMPUTATION OF THE ADIABATIC FLAME
            C          TEMPERATURE MOST BE POSTPONED UNTIL SOME FUEL IS AL-
            C          LOWED TO VAPORIZE.
            C
            C
 0055             CALL THERMO(TO,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
 0056             CALL TADB(NIND,NDEP,NCOMP,YO,XZO,Y,XZ,DELH,DELALP,B,GAMMA,
                 1            CPCOEF,CPAVG,GO,G,TO,TADAB,HEAT)
 0057             IF(MACRO.EQ.1) GO TO 5020
 0058             PRINT 500, TADAB
 0059             IF (MACRO .EQ. 0) GO TO 503
 0060             IF(NSPRAY.NE.0)GO TO 503
 0061         500 FORMAT (1H1, 58X, 'COMBUSTION/POLLUTION MODEL',// 64X, 'OUTPUT',
                 1        ' SUMMARY',// 57X, 28('*'),////T20, 'ADIABATIC FLAME ',
                 2        'TEMPERATURE FOR INLET GAS MIXTURE = ', F10.2, ' K',/)
 0062        5020 XFIN1=XINJ(1)
 0063             KINJ=0
 0064         502 CALL       MCRMIX(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
                 1                  GAMMA,YO,XZOLD,YNOO,YNO,G,T,TB,
                 2                  XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
                 3                  DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
          4                 MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
          5                 TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
          6                 PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
          7                NSPRAY,ICODE,SS,NT,MACRO)
      C
            IF(IBOMB.EQ.3)GO TO 35
      C
            IF (IBOMB .NE. 0) GO TO 40
       5030 IBOMB=0
            KPOINT=1
            IDBUG=0
            YN2=XZO(4)
            YO2=YO(1)
            YNOEQ=0.
            MACRO1=0
            X=XO
            CALL    CRSCTN(KPOINT,X,XPOINT,AREA,PERIM,A,S)
            CALL         SPEED(P,TO,GOLD,GO,YNOLD,DELTAX,A,YN2,YO2,YNOO,YNOEQ,
          1  SS,MACRO,MACRO1,YO,XZO,X,PRINT,XFINAL,QNCHRT,QNCHTP,AREA,KPOINT,
          2 KO,NIND,NDEP,XPOINT,PERIM,XOLD,XO,NOPT,KODE,PINT,IDBUG)
            IF(IBOMB.EQ.3)GO TO 35
            IF(IBOMB.NE.0)GO TO 40
        503 IF (KODE(4) .LE. 0) GO TO 50
            XFIN = XINJ(1)
            CALL         INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
          1                 GAMMA,YO,XZOLD,YNOO,YNO,G,T,TB,
          2                 XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
          3                 DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
          4                 MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
          5                 TSPEC,QSPEC,KODE,GO,P,TO,XO,XFIN,DELTAX,
          6                 PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
          7                NSPRAY,ICODE,SS,NT,MACRO)
            IF(IBOMB.NE.0) GO TO 40
            KINJ = 0
         35 KINJ = KINJ+1
            IF(KINJ .GT. KODE(4)) GO TO 40
            XO = XINJ(KINJ)
            TEST1=XO+3.*DELTAX
            KINJEC=1
            KPASSS=1
            SS=XO
            IF(KINJ .EQ. KODE(4)) GO TO 30
            XFIN = XINJ(KINJ +1)
      C
            XFIN1=XFIN
            GO TO 31
         30 XFIN = XFINAL
            XFIN1=XFIN
         31 CONTINUE
            G2 =GINJ(KINJ)
            T2 =TINJ(KINJ)
            DO 32 KK = 1,NIND
         32 Y2(KK) = YINJ(KK,KINJ)
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0102              DO 33 KK= 1,NDEP
0103           33 XZ2(KK) = XZINJ(KK,KINJ)
0104              YNO2 = YNOINJ(KINJ)
0105              TCOMB=TCOMBI(KINJ)
0106              CALL        MIX(G,Y,XZ,YNO,T,G2,Y2,XZ2,YNO2,T2,GO,YO,XZO,YNOO,TO,
                1                 NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
0107              IF(XZO(1).LE.1.E-7.AND.IBOMB.EQ.3)GO TO 5030
0108              IF(IBOMB.EQ.3)IBOMB=0
0109              IF(IBOMB.NE.0) GO TO 40
0110              CALL THERMO(TO,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
0111              CALL TADB(NIND,NDEP,NCOMP,YO,XZO,Y,XZ,DELH,DELALP,B,GAMMA,
                1          CPCOEF,CPAVG,GO,G,TO,TADAB,HEAT)
0112              PRINT 501, TADAB
0113          501 FORMAT(                              ////T20, 'ADIABATIC FLAME ',
                2          'TEMPERATURE FOR INLET GAS MIXTURE = ', F10.2, ' K',/)
0114              CALL        INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
                1                 GAMMA,YO,XZOLD,YNOO,YNO,G,T,TB,
                2                 XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
                3                 DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
                4                 MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
                5                 TSPEC,QSPEC,KODE,GO,P,TO,XO,XFIN,DELTAX,
                6                 PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
                7                NSPRAY,ICODE,SS,NT,MACRO)
0115              IF(IBOMB.NE.0) GO TO 40
0116              GO TO 35
0117           50 CONTINUE
            C******* CALL THE SUBROUTINE 'INTGRT' WHICH INTEGRATES THE MASS AND
            C        ENERGY BALANCE EQUATIONS DOWN THE REACTOR.
0118              CALL        INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
                1                 GAMMA,YO,XZOLD,YNOO,YNO,G,T,TB,
                2                 XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
                3                 DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
                4                 MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
                5                 TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
                6                 PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
                7                NSPRAY,ICODE,SS,NT,MACRO)
0119              GO TO 40
0120              END
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FORTRAN IV G LEVEL  20                 ADATA                                              PAGE 0001

 0001             SUBROUTINE ADATA(NIND,NDEP,NCOMP,B,GAMMA,YO,XZU,CPCOEF,DCOF,YNOO,
                 1                   CP,DCPDT,DELH,DHDT,RCON,HTC,XPOINT,AREA,PERIM,
                 2                   TWALL,TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
                 3                   PINT,XINJ,CINJ,TINJ,YINJ,XZINJ,YNOINJ,
                 4                   NOPT,TX,CPY,C,FO,F,A,QNCHRT,GNCHTP,TCOMB,TCOMBI,
                 5                   NSPRAY,ICODE,TB,MACRO)
 0002             DIMENSION B(NIND,NIND),GAMMA(NDEP,NIND),YO(NIND),XZO(NDEP)
 0003             DIMENSION CPCGEF(NCOMP,10), DCOF(NIND,14)
 0004             DIMENSION CP(NCCMP),DCPDT(NCOMP),DELH(NIND),DHDT(NIND)
 0005             COMMON /MACROI/GO1,TO1,P1,TCOMB1,YO1(2),XZO1(4),YNOO1,XPONT1(10),
                 1                 AREA1(10 ),PERIM1(10 ),TWALL1(10 ),TSPEC1(10 ),
                 2           QSPEC1(10 ),RECYCL,RECYCR,PART,YO2EQ1
 0006             CGMMON /AA/ HVAP
 0007             DIMENSION PRINT(8)
 0008             DATA PRINT/
                 1  'FUEL',' OIL',' MOD','EL  ',
                 2   'COAL',' DUS','T MO','DEL '/
 0009             DIMENSION XPOINT(10 ),AREA(10 ),PERIM(10 ),TWALL(10)
 0010             DIMENSION QSPEC(10)
 0011             DIMENSION TSPEC(10 ),KODE(NOPT)
 0012             DIMENSION HTC(3),   RCON(10)
 0013             DIMENSICN TX(20),CPY(20),C(4),FO(4),F(20,4),A(4,4)
 0014             DIMENSION XINJ(20),GINJ(20),TINJ(20),YINJ(NIND,20),XZINJ(NDEP,20)
 0015             DIMENSION YNOINJ(20)
 0016             DIMENSION QNCHRT(3), TCOMBI(20)
 0017             DIMENSION TITLE(20),ICODE(6)
 0018             DIMENSIGN WRITES(4,5)
 0019             CCMMON/AB/R(10),RHONV(10),NGROUP,NFNCTN,RHOP,AVGMW,
                 1          VP,      WDP(10),XNDP(10)
 0020             CCMMON /EE/ FUEL
 0021             COMMON/CD/YO2EQ
 0022             COMMON /IJ/ VAPF
 0023             DATA WRITES/ 'NOT ','SPEC','IFIE','D   ','SPEC','IFIE','D   ','
                 1 ',            ' FUE','L EX','PONE','NT  ',' CO ','EXPO','NENT','
                 2 ',            'CCMP','UTED',' FRO','M QR'/
 0024             XO =       .0
 0025             B(1,2)=-0.5
 0026             B(2,2)= 1.0
 0027             GAMMA(1,2)=  0.0
 0028             GAMMA(2,2)= -1.0
 0029             GAMMA(3,2)=  0.0
 0030             GAMMA(4,2)=  0.0
 0031             READ(5,5012,END=100) (TITLE(I),I=1,20)
 0032        5012 FORMAT (20A4)
 0033             PRINT 5013,(TITLE(I),I=1,20)
 0034        5013 FORMAT (1H1,T10, 'COMBUSTION/POLLUTION MODEL--- ',20A4 //)
 0035             READ(5,1013,END=100) KODE,NSPRAY,MACRO
 0036        1013 FORMAT(16I5)
 0037             N1 = KODE(1) + 1
 0038             N2 = KODE(2) + 1
 0039             IF (N2.EQ.3) N2=5
 0040             N3 = KODE(3) + 1
 0041             PRINT 3013, KODE(1), (WRITES(IX,N1),IX=1,4),
               1             KODE(2), (WRITES(IX,N2),IX=1,4),
               2             KODE(3), (WRITES(IX,N3),IX=1,4), KODE(4)
 0042         3013 FORMAT (T19, 'DECK 3347'
               1       / / T16, 'INPLT SUMMARY', / T10, 26('*'), //5X, 'CARD 1 ',
               2       '- OPTIONS', / 5X, 16('-'),//13X, I2, ' WALL TEMPERATURE ',
               3      'PROFILE ',4A4, /13X, I2,' GAS TEMPERATURE PROFILE ', 4A4,/
               4     13X, I2, ' HEAT FLUX PROFILE ', 4A4,/13X, I2, ' NO. OF SECON',
               5       'DARY INJECTION PTS.')
            C******  READ THE STOICHIOMETRIC COEFFICIENTS FOR THE FIRST REACTION.
 0043              READ(5,1000) GAMMA(1,1),B(1,1),GAMMA(2,1),GAMMA(3,1)
 0044         1000 FORMAT(7F10.3)
 0045              PRINT 3000, GAMMA(1,1), B(1,1), GAMMA(2,1), GAMMA(3,1)
 0046         3000 FORMAT (/ 5X, 'CARD 2 - STOICHIOMETRIC COEFFICIENTS (FUEL COMBUS',
               1     'TION)',/ 5X, 54('-'), // 7X, F10.3, ' FUEL COEFFICIENT',/
               2     7X, F10.3, ' O2 COEFFICIENT ',/ 7X, F10.3,' CO COEFFICIENT',
               3     / 7X, F10.3,' H2O COEFFICIENT')
 0047              B(1,1) = -B(1,1)
 0048              B(2,1) = 0.0
 0049              GAMMA(1,1) = -GAMMA(1,1)
 0050              GAMMA(4,1) = 0.
            C****** READ INITIAL MOLAR GAS VELOCITY,INITIAL TEMPERATURE AND
            C            PRESSURE.
 0051              IF (MACRO .EQ. 0) GO TO 500
 0052              READ(5,1000)  GO1,TO1,P1,TCOMB1
 0053              READ(5,1000) GO,TO,P,TCOMB
 0054              READ(5,1000) YO1,XZO1,YNOO1
 0055              REAC(5,1000) YO, XZO, YNOO
 0056              PRINT 3510,GO,TO,P,TCOMB,GO1,TO1,P1,TCOMB1
 0057         3510 FORMAT(/5X, 'CARD 3 - PHYSICAL CONDITIONS OF INLET GAS MIXTURE',
               1 / 5X, 49('-'), / 23X, '** FUEL LEAN **', /26X, 9('-'), //
               2 7X, F10.3,' FLOW RATE (G-MOLES/SEC)', / 7X, F10.3,' TEMPERATURE (
               3K)', / 7X, F10.3, ' PRESSURE(PSIA)',/ 7X, F10.3, ' ADIABATIC FLAME
               4 TEMPERATURE AT INLET (K)', //23X, '** FUEL RICH **', / 26X, 9('-'
               5),//
               6 7X, F10.3,' FLOW RATE (G-MOLES/SEC)', / 7X, F10.3,' TEMPERATURE (
               7K)', / 7X, F10.3, ' PRESSURE(PSIA)',/ 7X, F10.3, ' ADIABATIC FLAME
               8 TEMPERATURE AT INLET (K)')
 0058               PRINT 3520, YO, XZO, YNOO, YO1, XZO1, YNOO1
 0059         3520 FORMAT( / 5X, 'CARD 4 - INLET GAS COMPOSITION',/ 5X, 30('-'),//
               1       23X, '** FUEL LEAN **', / 26X, 9('-'), //
               1       7X, F10.3, ' MOLE FRACTION OF O2',/ 7X, F10.3, ' MOLE FRACT',
               2       'ION OF CO2',/ 7X, F10.3, ' MOLE FRACTION OF FUEL',/ 7X,
               3       F10.3,' MOLE FRACTION OF CO',/ 7X, F10.3, ' MOLE FRACTION',
               4       ' OF H2O',/ 7X, F10.3, ' MOLE FRACTION OF N2 ',/ 7X, F10.3,
               5       ' MOLE FRACTION OF NO', //
               6       23X, '** FUEL RICH **', / 26X, 9('-'), //
               7       7X, F10.3, ' MOLE FRACTION OF O2',/ 7X, F10.3, ' MOLE FRACT',
               8       'ION OF CO2',/ 7X, F10.3, ' MOLE FRACTION OF FUEL',/ 7X,
               9       F10.3,' MOLE FRACTION OF CO',/ 7X, F10.3, ' MOLE FRACTION',
               A       ' OF H2O',/ 7X, F10.3, ' MOLE FRACTION OF N2 ',/ 7X, F10.3,
               B       ' MOLE FRACTION OF NO')
 0060               GO TO 600
 0061          500 READ(5,1000) GO,TO,P,TCOMB
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0062          PRINT 3010, GO, TO, P,TCOMB
0063     3010 FORMAT (/5X, 'CARD 3 - PHYSICAL CONDITIONS OF INLET GAS MIXTURE',
         1     / 5X, 49('-'), // 7X, F10.3, ' FLOW RATE (G-MOLES/SEC)',/
         2     7X, F10.3,' TEMPERATURE (K)', / 7X, F10.3,' PRESSURE(PSIA)',
         3/7X,F10.3,' ADIABATIC FLAME TEMPERATURE AT INLET (K)')
      C******  READ THE INITIAL GAS COMPOSITION.
0064          READ(5,1000) YO,XZO,YNOO
0065          PRINT 3020, (YO(ID), ID=1,2), (XZO(JD), JD=1,4),YNOO
0066     3020 FORMAT (/ 5X, 'CARD 4 - INLET GAS COMPOSITION',/ 5X, 30('-'),//
         1     7X, F10.3, ' MOLE FRACTION OF O2',/ 7X, F10.3, ' MOLE FRACT',
         2     'ION OF CO2',/ 7X, F10.3, ' MOLE FRACTION OF FUEL',/ 7X,
         3     F10.3,' MOLE FRACTION OF CO',/ 7X, F10.3, ' MOLE FRACTION',
         4     ' OF H2O',/ 7X, F10.3, ' MOLE FRACTION OF N2 ',/ 7X, F10.3,
         5     ' MOLE FRACTION OF NO')
0067      600 IF(KODE(4).LE.0) GO TO 5
0068          KKKK = KODE(4)
0069          DO 6 IK = 1,KKKK
0070          READ(5,1000) GINJ(IK),TINJ(IK),XINJ(IK),TCOMBI(IK)
0071          PRINT 3030, GINJ(IK), TINJ(IK), XINJ(IK),TCOMBI(IK)
0072     3030 FORMAT (/5X, 'CARD 5 - CONDITION AND LOCATION OF SECONDARY INJEC',
         1     'TION GAS',/ 5X, 58('-'),// 7X, F10.3, ' FLOW RATE (G-MOLES',
         2     '/SEC)',/ 7X, F10.3, ' TEMPERATURE(K)',/ 7X, F10.3, ' INJEC',
         3     'TION POINT (FT.)',
         4/7X,F10.3,' ADIABATIC FLAME TEMPERATURE AT INJECTION POINT (K)')
0073          READ(5,1000)  ((YINJ(KR,IK),KR=1,NIND),(XZINJ(KR,IK),KR=1,NDEP),
         1                 YNOINJ(IK))
0074          PRINT 3040,  (YINJ(KR,IK), KR=1,NIND), (XZINJ(KR,IK), KR=1,NDEP),
         1                YNOINJ(IK)
0075     3040 FORMAT (/5X, 'CARD 6 - INJECTION GAS COMPOSITION',/5X, 34('-'),//
         1     7X, F10.3, ' MOLE FRACTION OF O2',/ 7X, F10.3, ' MOLE FRACT',
         2     'ION OF CO2',/ 7X, F10.3, ' MOLE FRACTION OF FUEL',/ 7X,
         3     F10.3, ' MOLE FRACTION OF CO',/ 7X, F10.3, ' MOLE FRACTION',
         4     ' OF H2O',/ 7X, F10.3, ' MOLE FRACTION OF N2',/ 7X, F10.3,
         5     ' MOLE FRACTION OF NO')
0076        6 CONTINUE
      C****** READ IN THE CONSTANTS IN THE FIRST RATE EXPRESSION. THE
0077        5 READ(5,1002) RCON
0078     1002 FORMAT(E10.2,4F10.3)
0079          PRINT 3002
0080     3002 FORMAT (/5X, 'CARD 7 - KINETIC RATE CONSTANTS FOR FUEL COMBUSTIO',
         1     'N',/5X, 51('-'),/)
0081          PRINT 3050, (RCON(IJ), IJ=1,4), (WRITES(IX,3), IX=1,4), RCON(5)
0082     3050 FORMAT ( 7X, E10.2, ' FREQUENCY FACTOR',/ 7X, F10.3, ' ACTIVATIO',
         1     'N ENERGY',/ 7X, F10.3,' O2 EXPONENT',/ 7X, F10.3, 4A4,/ 7X,
         2     F10.3, ' H2O EXPONENT')
0083          PRINT 4002
0084     4002 FORMAT (/5X, 'CARD 8 - KINETIC RATE CONSTANTS FOR CO COMBUSTION',
         1          /5X, 49('-'),/)
0085          PRINT 3050, (RCON(IJ), IJ=6,9), (WRITES(IX,4), IX=1,4), RCON(10)
0086          IF(KODE(1) .LE. 0) GO TO 7
      C****** READ IN THE HEAT TRANSFER COEFFICIENTS.
0087          READ(5,1000) HTC
0088          IF (KODE(1) .EQ. 1) PRINT 3060, (HTC(IL), IL=1,3)
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 3060 FORMAT (/5X, 'CARD 9 - HEAT TRANSFER CONSTANTS',/5X, 32('-'),//7X,
     1     F10.3, ' CONSTANT COEFFICIENT',/ 7X, F10.3, ' CONVECTION ',
     2     'COEFFICIENT',/ 7X, F10.3, ' RADIATION COEFFICIENT')
    7 IF(KODE(2).NE.2)  GO TO 8
      READ 1000, QNCHRT, QNCHTP
      PRINT 4000,QNCHRT
 4000 FORMAT (/5X,'CARD 9.5 - QUENCH RATE CONSTANTS',/5X,32('-'),//7X,
     1 F10.3,' FIRST COEFFICIENT'    ,/7X,F10.3,' SECOND COEFFICIENT',/
     2 7X,F10.3,' THIRD COEFFICIENT')
      IF(QNCHTP.EQ.0) PRINT 4001
 4001 FORMAT(/7X,'QUACRATIC RATE TO BE USED')
      IF(QNCHTP.EQ.1) PRINT 4003
 4003 FORMAT(/7X,'EXPONENTIAL RATE TO BE USED')
    8 CONTINUE
      KK = 0
      PRINT 1014
 1014 FORMAT (/5X, 'CARD 10 - COMBUSTOR PROFILES',/5X, 28('-'),//
     1         10X,'DISTANCE   CROSS-SECTIONAL AREA   PERIMETER   WALL TE
     1MPERATURE   GAS TEMPERATURE      HEAT FLUX',/11X,'(FEET)',12X,
     2'(FT2)',12X,'(FEET)',11X,'(K)',15X,'(K)',9X,'(KCAL/FT2-SEC)'/
     3 11X,6('-'),12X,5('-'),12X,6('-'),11X,3('-'),15X,3('-'),9X,14('-')
     5//)
   20 KK = KK+1
      IF (MACRO .EQ. 0) GO TO 700
      READ(5,1012) XPONT1(KK),AREA1(KK),PERIM1(KK),TWALL1(KK),
     1        TSPEC1(KK),QSPEC1(KK)
  700 READ(5,1012)XPOINT(KK),AREA(KK),PERIM(KK),TWALL(KK),TSPEC(KK),
     1QSPEC(KK),KCHECK
 1012 FORMAT(6F10.3,19X,I1)
      PRINT 3012, XPOINT(KK), AREA(KK), PERIM(KK), TWALL(KK), TSPEC(KK),
     1     QSPEC(KK)
 3012 FORMAT(8X,F10.3,8X,F10.3,8X,F10.3,5X,F10.3,8X,F10.3,9X,F10.3)
      IF(KCHECK.LE.0) GO TO 20
C******  READ IN REACTOR LENGTH AND PRINT INTERVAL.
      READ(5,1000) XFINAL,PINT,DELTAX
      PRINT 3070, XFINAL, PINT,DELTAX
 3070 FORMAT (/5X, 'CARD 11 - COMBUSTOR LENGTH AND PRINOUT INTERVAL',/
     1         5X, 47('-'),// 7X, F10.3, ' REACTOR LENGTH (FEET)',/ 7X,
     2         F10.3, ' PRINTOUT INTERVAL (FEET)',
     3 /7X,F10.3,'INTEGRATION INTERVAL (FEET)')
      TREF = 298.
C****    READ THE HEATS OF REACTION AT THE REFERENCE TEMPERATURE.
      READ(5,1000) (DCOF(IR,11),IR = 1,NIND)
      PRINT 3080, (DCOF(IR,11), IR= 1,NIND)
 3080 FORMAT (/5X, 'CARD 12 - HEAT OF REACTION AT 298K',/ 5X, 34('-'),//
     1     7X, F10.3, ' HEAT OF REACTION FOR FUEL COMBUSTION',/ 7X,
     2     F10.3, ' HEAT OF REACTION FOR CO COMBUSTION')
C     READ IN THE HEAT CAPACITY DATA FOR FUEL AND CURVE FIT IT.
C     WRITE(6,1010)
C1010 FORMAT(1H1,'HEAT CAPACITY DATA FOR   FUEL      IS FITTED BY THE FO
C    1LLOWING FUNCTION,'//,' FOR T .GE. 298K AND .LE. 1200K',/,' CP= A1
C    2+ A2*(T/1000.) + A3*(T/1000.)**2 + A4*(T/1000.)**3 + A5*(T/1000.)*
C    3*4',//,' FOR T .GT. 1200K',/,' CP= A6 + A7/(T/1000.) + A8/((T/1000
              C    4.)**2) + A9/((T/1000.)**3) + A10/((T/1000.)**4)',////)
 0117                KASE = 0
 0118                NCON = 4
 0119                READ(5,2000)NPTS,TI,CPI
 0120                PRINT 3090, NPTS, TI, CPI
 0121           3090 FORMAT (/5X, 'CARD 13 - HEAT CAPACITY DATA FOR FUEL (298K TO 1200K
                   1)',      / 5X, 53('-'), // 13X, I2,' NO. OF HEAT CAPACITY DATA',
                   2          ' POINTS FOR FUEL (298K TO 1200K)', // 5X, 'CARD 14 - HE',
                   3         'AT CAPACITY DATA POINTS FOR FUEL (298K TO 1200K)', / 5X,
                   4          60('-'),//7X, 'TEMPERATURE (K)', 4X, 'HEAT CAPACITY OF FU'
                   5         ,'EL (CAL/G-MOLES, K)',/7X, 15('-'), 4X, 37('-'),//10X,
                   6          F10.3, 20X, F10.3)
 0122                NPTS = NPTS - 1
 0123           2000 FORMAT(I4,/,4X,2F10.3)
 0124                CALL        CPFIT(NPTS,NCON,TI,CPI,TX,CPY,CO,C,FO,F,A,KASE)
              C      WRITE(6,2002)CO,C
              C2002 FORMAT(1H ,'COEFFICIENTS IN THE HEAT CAPACITY EQUATION FOR T L.E.
              C    11200K ARE,',//,8X,'A1',14X,'A2', 14X,'A3',14X,'A4',14X,'A5',/(5E16
              C    2.4)//////////)
 0125                CPCOEF(3,1) = CO
 0126                DO 18 KC = 1,4
 0127                KCC = KC + 1
 0128             18 CPCOEF(3,KCC) = C(KC)
 0129                KASE = 1
 0130                TI = 1200.
 0131                TR = 1.
 0132                CPI = CO
 0133                DO 1 KK= 1,NCON
 0134                TR  = TR *1.2
 0135              1 CPI = CPI+ C(KK)*TR
 0136                READ(5,1001) NPTS
 0137           1001 FORMAT(I4)
 0138                PRINT 3110, NPTS
 0139           3110 FORMAT (/5X, 'CARD 15 - HEAT CAPACITY DATA FOR FUEL (T > 1200K)',
                   1          /5X, 48('-'),//13X, I2, ' NO. OF HEAT CAPACITY DATA ',
                   2          'POINTS FOR FUEL (T > 1200K)',// 5X, 'CARD 16 - HEAT CAP',
                   3          'ACITY DATA POINTS FOR FUEL (T > 1200K)',/5X,54('-'),//7X,
                   4         'TEMPERATURE (K)', 4X, 'HEAT CAPACITY OF FUEL (CAL/G-MOLE',
                   5          'S,K)',/7X, 15('-'), 4X, 37('-'),/)
 0140                CALL       CPFIT(NPTS,NCON,TI,CPI,TX,CPY,CO.C.FO,F,A,KASE)
 0141                CPCOEF(3,6) = CO
 0142                DO 19 KC = 1,4
 0143                KCC = KC + 6
 0144             19 CPCOEF(3,KCC) = C(KC)
              C      WRITE(6,1004)CO,C
              C1004 FORMAT(1H ,'COEFFICIENTS IN THE HEAT CAPACITY EQUATION FOR T G.E.
              C    11200K ARE,',//,8X,'A6',14X,'A7', 14X,'A8',14X,'A9',14X,'A10',/(5E1
              C    26.4))
              C**** CALCULATE THE COEFFICIENTS IN THE DELTA CP EXPRESSION.
 0145                DO 10 IREAT = 1,NIND
 0146                DO 10 IC = 1,10
 0147                DCOF(IREAT,IC) = 0.
 0148                DO 9 IR = 1,NIND
```

```
          9 DCOF(IREAT,IC) = DCCF(IREAT,IC) + B(IR,IREAT)*CPCOEF(IR,IC)
            DO 10 IR=1,NDEP
            NC = IR + NIND
         10 DCOF(IREAT,IC) = DCOF(IREAT,IC) + GAMMA(IR,IREAT)*CPCOEF(NC,IC)
      C****    CALCULATE THE ADDITIONAL CONSTANTS NEEDED
            TR = TREF/1000.
            T1 = 1.
            DO 11  IR = 1,NIND
         11 DCOF(IR,13) = 0.
            DO 12 IC =1,5
            AC = IC
            T1 = T1*TR
            T2= T1/AC
            DO 12 IR =1,NIND
         12 DCOF(IR,13) = DCOF(IR,13) + DCOF(IR,IC) *T2
            DO 13 IR=1,NIND
         13 DCOF(IR,14) = 0.
            DO 14 IR = 1,NIND
         14 DCOF(IR,14) = DCOF(IR,6)*1.2
            T2 = ALOG(1.2)
            DO 15 IR = 1,NIND
         15 DCOF(IR,14) = DCOF(IR,14) + DCOF(IR,7)*T2
            T2 = 1.
            T1 = 1.0
            DO 16 IC = 8,10
            AC = IC - 7
            T1= T1/1.2
            T2= T1/AC
            DO 16 IR = 1,NIND
         16 DCOF(IR,14) = DCOF(IR,14) - DCOF(IR,IC)*T2
            T1 = 1.2
            T2 = T1*1.2
            T3 = T2*1.2
            T4 = T3*1.2
            T5 = T4*1.2
            DO 17 IR = 1,NIND
         17 DCOF(IR,12) = DCOF(IR,11) +       (DCOF(IR,1)*T1 + DCOF(IR,2)*T2/
           12. + DCOF(IR,3)*T3/3. + DCOF(IR,4)*T4/4. + DCOF(IR,5)*T5/5. -
           2 DCOF(IR,13))
            IF (MACRO .EQ. 0) GO TO 800
            READ 90, YO2EQ1
        800 READ 90,YO2EQ
         90 FORMAT(5E10.4)
            IF(YO2EQ.LE.0.)GO TO 93
            IF (MACRO .EQ. 0) GO TO 5090
            PRINT 3091, YO2EQ, YO2EQ1
       3091 FORMAT(//// 12X, 'THE EQUILIBRIUM MOLE FRACTION OF O2 IS ASSUMED T
           1O BE = ', E10.4, ' FOR FUEL LEAN', / 12X, 'THE EQUILIBRIUM MOLE FR
           2ACTION OF O2 IS ASSUMED TO BE = ', E10.4, ' FOR FUEL RICH')
            GO TO 93
       5090 PRINT 91,YO2EQ
         91 FORMAT(//// 12X,'THE EQUILIBRIUM MOLE FRACTION OF O2 IS ASSUMED TO
           1 BE=',E10.4)
```

```
 0196            93 IF (MACRO .EQ. 0) GO TO 94
 0197               READ 90, PART,RECYCL.RECYCR
 0198               PRINT 5590,RECYCL,RECYCR,PART
 0199          5590 FORMAT (//// 12X, 'FRACTION OF FUEL LEAN STREAM TRANSFERRED TO THE
                   1 RICH ZONE = ', E10.4, / 12X, 'FRACTION OF FUEL RICH STREAM TRANSF
                   2ERRED TO THE LEAN ZONE = ', E10.4, / 12X, 'FRACTION OF VOLUME IN F
                   3UEL LEAN ZONE = ', E10.4)
 0200            94 IF(NSPRAY.EQ.0)      RETURN
 0201               READ 25,(ICODE(I),I=1,NCOMP),NFNCTN,NGROUP,RHOP,AVGMW,FUEL,TB,
                   1      VAPF,HVAP
 0202            25 FORMAT(6I2,2I3,4F10.1,2E10.1)
 0203               N=NSPRAY
 0204               IF (NSPRAY .EQ. 2) N=5
 0205               NIX = N + 3
 0206               PRINT 6000,(PRINT(IX), IX = N, NIX),  NGROUP,AVGMW,RHOP,TB,VAPF,
                   1             HVAP
 0207          6000 FORMAT (/5X, 'CARD 18 - ', 4A4, / 5X, 25('-'),
                   1       // 12X, I3, ' PARTICLE SIZE DISTRIBUTION',
                   2        / 5X, F1C.1, ' MOLECULAR WEIGHT OF FUEL IN VAPOR STATE',
                   3        / 5X, F1C.1, ' DENSITY OF FUEL OIL DROPLETS',
                   4        / 5X, F1C.1, ' BOILING POINT OF FUEL OIL (OK)',
                   5        / 5X, E1C.1, ' VAPORIZATION CONSTANT (FT**2/SEC)',
                   6        / 5X, E10.1, ' HEAT OF VAPORIZATION (CAL/GM-MOLE)')
 0208               DO 22 I=1,NGROUP
 0209               READ 21,R(I),WOP(I)
 0210            21 FORMAT(2E10.1)
 0211            22 CONTINUE
 0212               RETURN
 0213           100 STOP
 0214               END
```

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FORTRAN IV G LEVEL  20                MCRMIX                                         PAGE 0001

 0001              SUBROUTINE MCRMIX(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YNOLD,Y,GAMBIV,B,
                  1                    GAMMA,YO,XZOLD,YNOO,YNO,G,T,TB,YOLD,
                  2                    XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
                  3                    DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
                  4                    MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL.
                  5               TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
                  6                    PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
                  7                    NSPRAY,ICODE,SS,NT,MACRO)
 0002         9990 CONTINUE
 0003              DIMENSION YR(2),XZR(4),YL(2),XZL(4)
 0004              DIMENSION DABINV(NIND),YO(NIND),Y(NIND),YOLD(NIND),YO(NIND)
 0005              DIMENSION GAMBIV(NDEP,NIND),XZOLD(NDEP)
 0006              DIMENSION B(NIND,NIND),XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
 0007              DIMENSION DCOF(NIND,14)
 0008              DIMENSION DGIDY(NIND),DXZDY(NDEP,NIND),R(NIND),DRDY(NIND,NIND)
 0009              DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
 0010              DIMENSION DGCPDY(NIND),DELH(NIND),DHDT(NIND),LMINV(NDIM)
 0011              DIMENSION MMINV(NDIM)
 0012              DIMENSION XZ(NDEP),AJACOB(NDIM,NDIM),FUN(NDIM)
 0013              DIMENSION XPOINT(1)  ,AREA(1)  ,PERIM(1)  ,TWALL(1)
 0014              DIMENSION TSPEC(1)  ,KODE(NOPT)
 0015              DIMENSION QSPEC(1)
 0016              DIMENSION QNCHRT(3)
 0017              DIMENSION GAMMA(NDEP,NIND)
 0018              DIMENSION HTC(3),RCON(10)
 0019              DIMENSION XMOLE(6),ICODE(6),XZ2(4),Y2(2), CPAVG(6)
 0020              DIMENSION YTEMP(2),XZTEMP(4),DUM1(2),DUM2(4)
 0021              COMMON /MACROI/G01,T01,P1,TCOMB1,YO1(2),XZ01(4),YNO01,XPONT1(10).
                  1              AREA1(10 ),PERIM1(10 ),TWALL1(10 ),TSPEC1(10 ),
                  2         QSPEC1(10 ),RECYCL,RECYCR,PART,YO2EQ1
 0022              COMMON /FLOOD/ MACRO1
 0023              COMMON /FLOOD1/ A,S,KPOINT,X
 0024              COMMON /POLMCR/DNODTT, VOLUME
 0025              COMMON /CD/ YO2EQ
 0026              COMMON/PRNT/XPRINT
 0027              QCON=0.95
 0028              IDBUG=0
 0029              XPRINT=0.
 0030              KPASL = 0
 0031              KPASR = 0
 0032              MACRO1 = 0
 0033              YO2EQL=YO2EQ
 0034              YO2EQR=YO2EQ1
 0035              YNOL = YNOO
 0036              X=XO
 0037              XOLD=X
 0038              TADABL=TADAB
 0039              KQUENC=0
 0040              SS = 0.0
 0041              YNOEQ=0.
 0042              CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,1,YNOEQ)
 0043              PRINT 5
 0044              CALL OUTONE(NIND,NDEP,X,GO,YO,XZO,YNOO,TO,2,YNOEQ)
```

```
      PRINT 6
      CALL OUTONE(NIND,NDEP,X,G01,Y01,XZ01,YNO01,T01,2,YNOEQ)
    5 FORMAT(//5X,' COMPOSITION OF FUEL LEAN STREAM '//)
    6 FORMAT(//5X,' COMPOSITION OF FUEL RICH STREAM '//)
      MRICH = 0
      MM = 0
      TGUESL=0.
      TGUESR=0.
      KPOINT = 1
C
C      FIRST STEP IS TO COMPUTE THE COMPOSITION OF THE FUEL LEAN STREAM
C
C--------------INITIALIZATION
C
    7 CALL       CRSCTN(KPOINT,X,XPOINT,AREA,PERIM,A,S)
      AL=A*PART
      AR=A*(1.-PART)
      SL=S*PART
      SR=S*(1.-PART)
      DO 20 I=1,NIND
      Y2(I) = Y0(I)
   20 CONTINUE
      DO 25 I=1,NDEP
      XZ2(I)=XZ0(I)
   25 CONTINUE
      T2 = T0
      G2 = G0
      YNO2 =  YNO0
      A=AL
      S=SL
C
C      COMPUTE FUEL LEAN FIRST
C
   35 CALL INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,Y2,YOLD,Y,GAMBIV,B,
     1           GAMMA,Y0,XZOLD,YNO2,YNO,G,T,TB,
     2           XZ2,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
     3           DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
     4           MMINV,XZ,AJACOB,FUN,XPONT1,AREA1,PERIM1,TWALL1,
     5           TSPEC1,QSPEC1,KODE,G2,P1,T2,X0,XFINAL,DELTAX,
     6           PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
     7           NSPRAY,ICODE,SS,NT,MACRO)
      IF (IBOMB .NE. 0) RETURN
      IF (MACRO .EQ. 3) MACRO1=1
      IF (MRICH .EQ. 1) GO TO 90
      IF (MM .EQ. 0) GO TO 70
C
C      CHECK CONVERGENCE
C
      ADIST = 0.
      DO 40 I=1,NIND
      YNOW = Y(I)
      YPREV = YL(I)
      YL(I)=YNOW
```

```
          HOLD =(ABS(YNOW-YPREV))/YPREV
          IF (HOLD .GT. ADIST) ADIST=HOLD
       40 CONTINUE
          TNOW=T
          TPREV=TL
          HOLD=(ABS(TNOW-TPREV))/TPREV
          IF(HOLD.GT.ADIST)ADIST=HOLD
C
C         STORE VALUES OF COMPOSITION OF FUEL LEAN-RECYCLE STREAM
C
       70 TL=T
          GREL=G*RECYCL
          GL=G
          G=GL-GREL
          TGUESL=T
          IF(IDBUG.EQ.0)GO TO 74
          PRINT 5
          CALL OUTONE(NIND,NDER,X,G,Y,XZ,YNO,T,2,YNOEQ)
       74 IF(MM.GE.1)GO TO 76
          DO 75 I=1,NIND
          YL(I) = Y(I)
       75 CONTINUE
       76 DO 77 I=1,NDEP
          XZL(I) = XZ(I)
       77 CONTINUE
          IF (MM .EQ. 0) GO TO 78
          IF (ADIST .LT. .001) GO TO 180
       78 MRICH=1
          A=AR
          S=SR
C
C         MIX FUEL RICH STREAM WITH FUEL LEAN RECYCLE
C
          CALL MIX(G01,Y01,XZ01,YNO01,T01,GREL,YL,XZL,YNOL,TL,G2,Y2,XZ2,
         1      YNO2,T2,NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
          YNOR = YNO2
       79 CALL TADB(NIND,NDEP,NCOMP,Y2,XZ2,DUM1,DUM2,DELH,DELALP,B,GAMMA,
         1   CPCOEF,CPAVG,G2,DUM3,T2,TADAB,HEAT)
C
C          GO TO 35 TO COMPUTE FUEL RICH STREAM WITH RECYCLED FUEL LEAN GAS
C
          GO TO 35
C
C         STORE VALUES OF COMPOSITION, TEMPERATURE AND FLOWRATE OF FUEL RICH
C              RECYCLE STREAM
C
       90 MRICH = 0
          A=AL
          S=SL
          GRER=G*RECYCR
          GR=G
          G=GR-GRER
          IF(IDBUG.EQ.0)GO TO 91
          PRINT 6
          CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,2,YNOEQ)
       91 TR=T
          DO 150 I=1,NIND
          YR(I) = Y(I)
      150 CONTINUE
          DO 155 I=1,NDEP
          XZR(I) = XZ(I)
      155 CONTINUE
          CALL MIX(GO,YO,XZO,YNOO,TO,GRER,YR,XZR,YNOR,TR,G2,Y2,XZ2,YNO2,
         1      T2,NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
          YNOL=YNO2
          MM = MM+1
          GO TO 79
C
C-------- GET READY TO TAKE ANOTHER INTEGRATION STEP
C
      180 MRICH=0
          ADIST=1.
          MM = 0
          GOLDL=GO+GRER
          GOLDR=GO1+GREL
          GO=GL-GREL
          GO1=GR-GRER
          YNOLDL = YNOL
          YNOLDR = YNOR
          MACRO1 =0
C
C         COMPUTE THE NITROGEN OXIDE CONCENTRATION OF THE FUEL LEAN STREAM
C
          YO2L=YL(1)
          IF (YO2L .GT. YO2EQL .OR. KPASL .GT. 0) GO TO 188
          KPASL = 1
          IF (YO2EQL .EQ. 0) YO2EQL = YO2L
          YO2L = YO2EQL
          YO2EQL=0.
      188 YN2L = XZL(4)
          CALL POLUT(P,TL,GOLDL,GL,YNOLDL,DELTAX,AL,YN2L,YO2L,YNOL,YNOEQL,SS
         1      ,MACRO)
          REDUC = DNODTT * VOLUME/GL/2.
          YO2L = YO2L - REDUC
          YL(1) = YO2L
          YN2L = YN2L - REDUC
          XZL(4) = YN2L
C
C          COMPUTE NO CONCENTRATION OF THE FUEL RICH STREAM
C
          YO2R=YR(1)
          IF (YO2R .GT. YO2EQR .OR. KPASR .GT. 0) GO TO 205
          KPASR = 1
          IF (YO2EQR .EQ. 0) YO2EQR =YO2R
          YO2R = YO2EQR
          YO2EQR=0.
```

```
 0160          205 YN2R = XZR(4)
 0161              CALL POLUT(P,TR,GOLDR,GR,YNOLDR,DELTAX,AR,YN2R,YO2R,YNOR,YNOEQR,
                  1      SS,MACRO)
 0162              REDUC = DNODTT * VOLUME / GR/ 2.
 0163              YO2R = YO2R-REDUC
 0164              YR(1)=YO2R
 0165              YN2R = YN2R-REDUC
 0166              XZR(4) = YN2R
 0167              CALL NORMA(GL,XZL,YL,YNOL,NIND,NDEP)
 0168              CALL NORMA(GR,XZR,YR,YNOR,NIND,NDEP)
               C
               C     GET READY TO TAKE ANOTHER INTEGRATION STEP
               C
 0169              XO=SS
 0170              XOLD=XO
 0171              SS=SS+DELTAX
 0172              X=SS
 0173              MACRO=2
 0174              DO 400 I=1,NIND
 0175              YO(I)=YL(I)
 0176              YO1(I)=YR(I)
 0177          400 CONTINUE
 0178              DO 410 I=1,NDEP
 0179              XZO(I)=XZL(I)
 0180              XZO1(I)=XZR(I)
 0181          410 CONTINUE
 0182              YNOO=YNOL
 0183              YNOO1=YNOR
               C   IF(X.LT.XPRINT)GO TO 412
 0184              PRINT 5
 0185              CALL OUTONE(NIND,NDEP,X,GO,YL,XZL,YNOL,TL,2,YNOEQL)
 0186              PRINT 6
 0187              CALL OUTONE(NIND,NDEP,X,GO1,YR,XZR,YNOR,TR,2,YNOEQR)
 0188          412 IF(KQUENC.GT.0)GO TO 425
 0189              IF(T.LT.(QCON*TADABL))GO TO 449
               C
               C        CHECK FOR QUENCHING
               C
 0190              MACRO1 = 0
 0191              KQUENC=1
 0192              KODE(1)=0
 0193              KODE(2)=2
 0194          425 TCOMB=TL
 0195              MACRO=3
               C
               C        QUENCH FUEL LEAN STREAM
               C
 0196              CALL QUENCH(TCOMB,X,XOLD,GL,P,AL,QNCHRT,QNCHTP,TL)
               C
               C        QUENCH FUEL RICH STREAM
               C
 0197              TCOMB=TR
 0198              CALL QUENCH(TCOMB,X,XOLD,GR,P,AR,QNCHRT,QNCHTP,TR)
```

```
      449 CONTINUE
          TO=TL
          TO1=TR
C
C-------- CHECK FOR COMPLETE MIXING
C
          IF (YL(1) .GT. YR(1)) GO TO 450
          RATIO=YR(1)/YL(1)
          GO TO 451
      450 RATIO=YL(1)/YR(1)
      451 IF(RATIO .LT.1.01)GO TO 459
      452 IF(SS.GT.XFINAL)GO TO 999
C
C-----IF FUEL IS LESS THAN 1.E-7, THERE IS NO NEED TO CONTINUE REACTING
C     THE MIXTURE.  THEREFORE, PROCEED TO BACMIX SUBROUTINE.  BACMIX IS
C     A TRIAL AND ERROR MIXING OF STREAM WITH NO CHEMICAL REACTIONS.
C
          DO 458 I=1,NDEP
          II=I+NIND
          IF (ICODE(II) .EQ. 0) GO TO 458
          IF (XZR(I) .LT. 1.E-7) GO TO 600
      458 CONTINUE
          GO TO 7
C
C     FUEL RICH AND FUEL LEAN STREAMS ARE MERGED
C
      459 PRINT 460
      460 FORMAT(//// 10X,'FUEL RICH AND FUEL LEAN STREAM HAVE MERGED IN MCR
         1MIX'////)
          GL=GO
          GR=GO1
          X=SS
          CALL MIX(GL,YL,XZL,YNOL,TL,GR,YR,XZR,YNOR,TR,GO,YO,XZO,YNOO,TO,
         1        NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
          CALL OUTONE(NIND,NDEP,X,GO,YO,XZO,YNOO,TO,2,YNOEQL)
          PRINT 461
      461 FORMAT(1HO)
          MACRO=2
          MACRO1=1
          IF(XZR(1).GT.1.E-4)RETURN
      600 PRINT 601
      601 FORMAT(//1X, 'FUEL IS EXHAUSTED--PROCEED TO MIX WITH NO COMBUSTION
         1 REACTIONS'//)
          CALL         BACMIX(TO,TL,TO1,TR,YL,YO,XZL,XZO,YR,YO1,XZR,XZO1,
         1   GO,GO1,GR,GL,RECYCR,RECYCL,YNOO,YNOL,  YNOO1,YNOR,  CPAVG,
         2   CPCOEF,NIND,NDEP,NCOMP,XFINAL,P,GCLDR,GOLDL,DELTAX,AR,SS,
         3   MACRO,AL,GRER,GREL,IBOMB,IDBUG,X,YO2EQL,YO2EQR,YNOEQL,XO,
         4   KPOINT,XPOINT,AREA, PERIM,QNCHRT,QNCHTP,KO,PART,PINT,ICODE,
         5   KODE,NOPT,XOLD)
          IF (IBOMB .NE. 0 ) RETURN
          RETURN
      999 CONTINUE
          PRINT 1020
```

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 0233         1020 FORMAT(1X,'THE END OF THE REACTOR HAS BEEN REACHED WHILE MIXING')
 0234              IBOMB=1
 0235              RETURN
 0236              END
```

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FORTRAN IV G LEVEL  20                  BACMIX                                                  PAGE 0001

0001                  SUBROUTINE BACMIX(TO,TL,TO1,TR,YL,YO,XZL,XZO,YR,YO1,XZR,XZO1,
                     1   GO,GO1,GR,GL,RECYCR,RECYCL,YNOO,YNOLDL,YNOO1,YNOLDR,CPAVG,
                     2   CPCOEF,NIND,NDEP,NCOMP,XFINAL,P,GOLDR,GOLDL,DELTAX,AR,SS,
                     3   MACRO,AL,GRER,GREL,IBOMB,IDBUG,X,YO2EQL,YO2EQR,YNOEQL,XO,
                     4   KPOINT,XPOINT,AREA, PERIM,QNCHRT,QNCHTP,KO,PART,PINT,ICODE,
                     5   KODE,NOPT,XOLD)
               C
               C
               C
0002                  DIMENSION YR(2),XZR(4),YL(2),XZL(4),YLPREV(2)
0003                  DIMENSION YO(NIND),XZO(NDEP),YO1(2),XZO1(4),CPAVG(6),
                     1        CPCOEF(NCOMP,10),KODE(NOPT),QNCHRT(3),ICODE(6)
0004                  DIMENSION XPOINT(1)  ,AREA(1)  ,PERIM(1)  ,TWALL(1)
0005                  COMMCN /POLMCR/DNODTT, VOLUME
0006                  COMMON /FLOGD/ MACRO1
0007                  COMMON/PRNT/XPRINT
0008                  COMMON/CD/YO2EQ
               C
               C
               C
               C-------- THIS SUBROUTINE BECOMES THE EXECUTIVE PROGRAN WHEN
               C          CHEMICAL REACTIONS CEASE .  THIS SUBROITINE MIXES THE STREAM AND
               C          SETIS UP THE TRIAL AND ERROR.
               C
0009                  IBOMB=0
0010             9990 CONTINUE
0011                  IF(KODE(1).EQ.2) GO TO 1
0012                  IF(KODE(2).EQ.2) GO TO 1
0013                2 CONTINUE
               C
               C      THIS SPACE IS RESERVED FOR FUTURE INCORPORATICN OF OTHER OPTIONS
               C
0014                1 IF (KODE(1).EQ.2)KODE(2)=2
0015                  IF(KODE(1).EQ.2)KODE(1)=0
0016                7 M1=0
0017                5 FORMAT(//5X,' CCMPOSITION OF FUEL LEAN STREAM '//)
0018                6 FORMAT(//5X,' CCMPOSITION OF FUEL RICH STREAM '//)
0019                  CALL       CRSCTN(KPOINT,X,XPOINT,AREA,PERIM,A,S)
0020                  AL=A*PART
0021                  AR=A*(1.-PART)
                      PART=FRACTION OF STREAM THAT IS FUEL LEAN
0022                  X=SS
               C
                      QUENCH FUEL LEAN STREAM
               C
0023                  CALL QUENCH(TO,X,XOLD,GL,P,AL,QNCHRT,QNCHTP,TL)
0024                  TO=TL
               (          QUENCH FUEL  RICH STREAM
               C
0025                  CALL QUENCH(TO1,X,XOLD,GR,P,AR,QNCHRT,QNCHTP,TR)
0026                  TO1=TR
0027                8 DO 9 I=1,NIND
0028                  YLPREV(I)=YL(I)
```

```
FORTRAN IV G LEVEL  20                BACMIX                                          PAGE 0002

0029          9 CONTINUE
0030            ADIST=1.
0031            TLPREV=TL
          C
          C     MIX FUEL LEAN STREAM WITH FUEL RICH RECYCLE
          C
0032            CALL MIX(GO,YO,XZO,YNOO,TO,GRER,YR,XZR,YNOLDR,TR,GL,YL,XZL,
               1         YNOLDL,TL,NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
0033            IF(IBOMB.NE.0)RETURN
0034            IF(M1.EQ.0)GO TO 70
0035            ADIST = 0.
0036            DO 40 I=1,NIND
0037            HOLD= ABS(YL(I)-YLPREV(I))/YLPREV(I)
0038            YLPREV(I)=YL(I)
0039            IF(HOLD.GT.ADIST)ADIST=HOLD
0040         40 CONTINUE
0041            HOLD=(ABS(TLPREV-TL))/TLPREV
0042            IF(HOLD.GT.ADIST)ADIST=HOLD
          C
          C          STORE VALUES OF EXIT COMPOSITION OF FUEL LEAN STREAM
          C          FOR THIS ITERATION.
          C
0043         70 TLPREV=TL
0044            GREL=GL*RECYCL
          C     GREL=MOLES CF LEAN STREAM RECYCLED TO FUEL RICH STREAM
0045            IF(IDBUG.EQ.0)GC TO 80
0046            PRINT 72,M1
0047         72 FORMAT(/1X,'FUEL LEAN STREAM',5X,I2)
0048            CALL OUTONE(NIND,NDEP,X,GL,YL,XZL,YNOLDL,TL,2,YNOEQL)
          C
          C          CHECK FOR CCNVERGENCE OF SUCCESIVE SUBSTITUTION
          C
0049         80 IF(ADIST.LT..C01)GO TO 180
          C
          C     MIX FUEL LEAN STREAM WITH FUEL LEAN RECYCLE
          C
0050            CALL MIX(G01,Y01,XZ01,YNO01,T01,GREL,YL,XZL,YNOLDL,TL,GR,YR,XZR,
               1         YNOLDR, TR,NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
0051            IF(IBOMB.NE.0)RETURN
0052            GRER=GR*RECYCR
          C     GRER=MOLES OF FUEL RICH STREAM RECYCLED TO FUEL LEAN STREAM
          C     RECYCL=FRACTION OF FUEL LEAN RECYCLED
          C     RECYCR=FRACTION OF FUEL RICH STREAM RECYCLED
0053            IF(IDBUG.EQ.0)GO TO 85
0054            PRINT 83,M1
0055         83 FORMAT(/1X,'FUEL RICH STREAM',5X,I2/)
0056            CALL OUTONE(NIND,NDEP,X,GR,YR,XZR,YNOLDR,TR,2,YNOEQR)
0057         85 M1=M1+1
0058            GO TO 8
0059        180 M1=0
0060            ADIST=1.
0061            GOLDL = GO + GRER
0062            GOLDR = G01 + GREL
```

```
0063            GO1=GR-GRER
0064            GO=GL-GREL
          C
          C         COMPUTE NITROGEN OXIDE CONCENTRATION FOR FUEL LEAN STREAM
          C
0065            YO2L=YL(1)
0066            IF (YO2L .LT.YO2EQL) YO2L=YO2EQL
0067            YN2L = XZL(4)
0068            CALL POLUT(P,TL,GOLDL,GL,YNOLDL,DELTAX,AL,YN2L,YO2L,YNOL,YNOEQL,SS
               1       ,MACRO)
0069            YNOLDL = YNOL
0070            IF (YO2L .GT. YO2EQL) GO TO 200
0071            YO2EQL=YO2EQL-DNODTT*VOLUME/GL/2.
0072            YO2L=YO2EQL
0073            GO TO 210
0074        200 REDUC=DNODTT*VOLUME/GL/2.
0075            YO2L=YO2L-REDUC
0076        210 YL(1)=YO2L
0077            YN2L=YN2L-REDUC
0078            XZL(4)=YN2L
          C
          C        COMPUTE NO CONCENTRATION OF THE FUEL RICH STREAM
          C
0079            YO2R=YR(1)
0080            IF (YO2R .LT.YO2EQR) YO2R=YO2EQR
0081            YN2R=XZR(4)
0082            CALL POLUT(P,TR,GOLDR,GR,YNOLDR,DELTAX,AR,YN2R,YO2R,YNOR,YNOEQR,
               1          SS,MACRO)
0083            YNOLDR = YNOR
0084            IF(YO2R .GT. YO2EQR)GO TO 300
0085            YO2EQR=YO2EQR-DNODTT*VOLUME/GR/2.
0086            YO2R=YO2EQR
0087            GO TO 310
0088        300 REDUC=DNODTT*VOLUME/GR/2.
0089            YO2R=YO2R-REDUC
0090        310 YR(1)=YO2R
0091            YN2R=YN2R-REDUC
0092            XZR(4)=YN2R
0093            XOLD=SS
0094            XO=SS
0095            SS=SS+DELTAX
0096            X=SS
          C
          C        GET READY TO TAKE ANOTHER INTEGRATION STEP
          C
0097            MACRO=2
0098            DO 400 I=1,NIND
0099            YO(I)=YL(I)
0100            YO1(I)=YR(I)
0101        400 CONTINUE
0102            DO 410 I=1,NDEP
0103            XZO(I)=XZL(I)
0104            XZO1(I)=XZR(I)
```

```
FORTRAN IV G LEVEL  20                BACMIX                                              PAGE 0004
       410 CONTINUE
           TO=TL
           TO1=TR
           YNOO=YNOL
           YNOO1=YNOR
           IF (YL(1) .GT. YR(1)) GO TO 450
           RATIO=YR(1)/YL(1)
           GO TO 451
       450 RATIO=YL(1)/YR(1)
       451 IF(RATIO .LT.1.01)GO TO 459
           IF(X.LT.XPRINT)GO TO 452
           PRINT 5
           CALL OUTONE(NIND,NDEP,X,GO,YL,XZL,YNOL,TL,2,YNOEQL)
           PRINT 6
           CALL OUTONE(NIND,NDEP,X,GO1,YR,XZR,YNOR,TR,2,YNOEQR)
           XPRINT=XPRINT+PINT
       452 IF(SS.GT.XFINAL)GO TO 999
           GO TO 7
     C
     C     FUEL RICH AND FUEL LEAN STREAMS ARF MERGED
     C
       459 PRINT 460
       460 FORMAT(//// 10X,'FUEL RICH AND FUEL LEAN STREAM HAVE MERGED'////)
           GL=GO
           GR=GO1
           CALL MIX(GL,YL,XZL,YNOL,TL,GR,YR,XZR,YNOR,TR,GO,YO,XZO,YNOO,TO,
          1       NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
           CALL OUTONE(NIND,NDEP,X,GO,YO,XZO,YNOO,TO,2,YNOEQL)
           A=AR+AL
           CALL       SPEED(P,TO,GOLD,GO,YNOLD,DELTAX,A,YN2,YO2,YNOO,YNOEQ,
          1  SS,MACRO,MACRO1,YO,XZO,X,PRINT,XFINAL,QNCHRT,QNCHTP,AREA,KPOINT,
          2 KO,NIND,NDEP,XPOINT,PERIM,XOLD,XO,NOPT,KODE,PINT,IDBUG)
           PRINT 461
       461 FORMAT(1HO)
           YO2EQ=YO2
           MACRO=0
           MACRO1=3
           IBOMB=1
           RETURN
       999 CONTINUE
           PRINT 1020
      1020 FORMAT(1X,'THE END OF THE REACTOR HAS BEEN REACHED WHILE MIXING')
           IBOMB=1
           RETURN
           END
```

```
FORTRAN IV G LEVEL  20                SPEED                                                      PAGE 0001
0001                  SUBROUTINE SPEED(P,TO,GOLD,GO,YNOLD,DELTAX,A,YN2,YO2,YNOO,YNOEQ,
                     1  SS,MACRO,MACRO1,YO,XZO,X,PRINT,XFINAL,QNCHRT,QNCHTP,AREA,KPOINT,
                     2 KO,NIND,NDEP,XPOINT,PERIM,XOLD,XO,NOPT,KODE,PINT,IDBUG)
                C
                C
                C          THE PURPOSE OF THIS SUBROUTINE IS TO SPEED-UP THE COM-
                C          PUTATIONS AFTER THE COMBUSTION REACTIONS ARE FROZEN.
                C          THEREFORE, THIS SUBROUTINE INTEGRATES THE NOX EQUATIONS
                C          ONLY. IN ADDTION, IT KEEPS TRACT OF THE OXYGEN DEPLE-
                C          TION DUE TO NITROGEN OXIDE REACTION.  THIS SUBROUTINE
                C          IS ACTIVATED AFTER ALL THE MIXING HAS CEASED.
                C
                C
0002                  DIMENSICN KODE(NOPT)
0003                  DIMENSION YO(NIND),XZO(NDEP),QNCHRT(3),AREA(1),XPOINT(1),PERIM(1)
0004                  CCMMCN /PCLMCR/ DNODTT,VOLUME
0005                  COMMCN/PRNT/XPRINT
0006                  CCMMON/INJECT/XFIN1
0007                  SS=X
0008                  XPRINT=X
0009                  XOLD=X
0010                  STEP=DELTAX
0011                  DIF=DELTAX
0012                  SS=SS+DELTAX
0013                  X=SS
0014                  XFIN2=XFINAL
0015                  IF(KODE(4).GT.0) XFINAL=XFIN1
0016                  YNOLD = YNOO
0017                  GOLD = GO
0018                  MACRO = 2
0019                  YO2 = YO(1)
0020                  YN2 = XZO(4)
0021                  TCCMB = TO
0022                5 CALL POLUT(P,TO,GOLD,GO,YNOLD,DELTAX,A,YN2,YO2,YNOO,YNOEQ,SS,
                    1 MACRO)
0023                  YNOLD = YNOO
0024                  REDUC = DNODTT * VOLUME/GO/2.
0025                  YO2 = YO2 - REDUC
0026                  YN2 = YN2 - REDUC
                C
                C      QUENCH
                C
0027                  CALL QUENCH (TCCMB,X,XOLD,GO,P,A,QNCHRT,QNCHTP,TO)
0028                  TCOMB = TO
0029                  YO(1) = YO2
0030                  XZO(4) = YN2
0031                  XOLD = X
                C
                C---------CHECK FOR INJECTICN POINT OR END OF REACTOR
                C           ADJUST STEP SIZE ACCORDINGLY.
                C
0032                  IF(DIF.EQ.0.) GO TO 20
0033                  DIF=XFINAL-XOLD
```

```
FORTRAN IV G LEVEL  20                   SPEED
                                                                                     PAGE 0002
 0034            IF(DIF.GT.DELTAX)GO TO 8
 0035            DELTAX=DIF
 0036            DIF=0.
 0037          8 SS=SS + DELTAX
 0038            X = SS
 0039            CALL       CRSCTN(KPOINT,X,XPOINT,AREA,PERIM,A,S)
 0040            IF(XOLD.LT.XPRINT)GO TO 5
 0041            CALL OUTONE(NIND,NDEP,XOLD,GO,YO,XZO,YNOO,TO,2,YNOEQ)
 0042            XPRINT=XPRINT+PINT
 0043            GO TO 5
 0044         20 IF(KODE(4).GT.0)GO TO 40
 0045         21 CALL OUTONE(NIND,NDEP,XFINAL,GO,YO,XZO,YNOO,TO,2,YNOEQ)
 0046            PRINT 22
 0047         22 FORMAT(/1X' THE END OF THE REACTOR HAS BEEN REACHED')
 0048            IBOMB=1
 0049            RETURN
           C
           C     DECIDE WHETHER OR NOT WE HAVE AN INJECTION POINT
           C
 0050         40 XFINAL=XFIN2
 0051            IF(XFIN1.GE.XFIN2)GO TO 21
 0052            IBOMB=3
 0053            DELTAX=STEP
 0054            CALL OUTONE(NIND,NDEP,XFIN1,GO,YO,XZO,YNOO,TO,2,YNOEQ)
 0055            PRINT 50
 0056         50 FORMAT(/1X,' INJECTION POINT HAS BEEN ENCOUNTERED---EXECUTION IS R
                1ETURNED TO MAIN'/)
 0057            RETURN
 0058            END
```

```
FORTRAN IV G LEVEL  20                  NORMA                                        PAGE 0001
                 SUBROUTINE NORMA(G,XZ,Y,YNO,NIND,NDEP)
                 DIMENSION XZ(4),Y(2)
                 DOUBLE PRECISION XZZ(4),YY(2),GY(2),GXZ(4),GG,SUM,GYNO,YYNO
      C
      C  THIS SUBROUTINE NORMALIZES THE CONCENTRATION OF THE FLOWING STREAM
      C
                 YYNO = YNO
                 DO 10 I=1,NIND
                 YY(I) = Y(I)
              10 CONTINUE
                 DO 20 I=1,NDEP
                 XZZ(I) = XZ(I)
              20 CONTINUE
                 GG = G
                 SUM = 0.
                 DO 30 I=1,NIND
                 GY(I) = GG * YY(I)
                 SUM = SUM + GY(I)
              30 CONTINUE
                 DO 40 I=1,NDEP
                 GXZ(I) = GG * XZZ(I)
                 SUM = SUM + GXZ(I)
              40 CONTINUE
                 GYNO = GG * YYNC
                 SUM = SUM + GYNO
                 G = SUM
                 YNO = GYNO/SUM
                 DO 50 I=1,NIND
                 Y(I) = GY(I)/SUM
              50 CONTINUE
                 DO 60 I=1,NDEP
                 XZ(I) = GXZ(I)/SUM
              60 CONTINUE
                 RETURN
                 END
```

```
FORTRAN IV G LEVEL  20                 CRSCTN                                                    PAGE 0001

        SUBROUTINE CRSCTN(KPOINT,X,XPOINT,AREA,PERIM,A,S)
        DIMENSION XPOINT(1),AREA(1),PERIM(1)
        IF(KPOINT.GT.1)GO TO 10
      9 KPOINT=KPOINT+1
        KC=KPOINT-1
     10 IF(X.GT.XPOINT(KPOINT))GO TO 9
        THTA=(X-XPOINT(KO))/(XPOINT(KPOINT)-XPOINT(KO))
        A=AREA(KO)+THTA*(AREA(KPOINT)-AREA(KO))
        S=PERIM(KO)+THTA*(PERIM(KPOINT)-PERIM(KO))
        RETURN
        END
      SUBROUTINE INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YU,YOLD,Y,GAMBIV,B,
     1                  GAMMA,YO,XZOLD,YNOO,YNO,G,T,TB,
     2                  XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
     3                  DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
     4                  MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
     5                  TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
     6                 PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
     7                 NSPRAY,ICODE,SS,NT,MACRO)
      DIMENSION DABINV(NIND),YO(NIND),Y(NIND),YOLD(NIND),YO(NIND)
      DIMENSION GAMBIV(NDEP,NIND),XZOLD(NDEP)
      DIMENSION B(NIND,NIND), XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
      DIMENSION DCOF(NIND,14)
      DIMENSICN DGIDY(NIND),DXZDY(NDEP,NIND),R(NIND),DRDY(NIND,NIND)
      DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
      DIMENSION DGCPDY(NIND),DELH(NIND),DHDT(NIND),LMINV(NDIM)
      DIMENSION MMINV(NDIM)
      DIMENSION XZ(NDEP),AJACOB(NDIM,NDIM),FUN(NDIM)
      DIMENSION XPOINT(2)  ,AREA(2)  ,PERIM(2)  ,TWALL(2)
      DIMENSION TSPEC(2)  ,KODE(NOPT)
      DIMENSION QSPEC(2)
      DIMENSION QNCHRT(3)
      DIMENSION GAMMA(NDEP,NIND)
      DIMENSION HTC(3),   RCON(10)
      DIMENSION XMOLE( 6),ICODE( 6),XZ2(4),Y2(2),CPAVG(6)
      DIMENSION YTEMP(2), XZTEMP(4)
      CCMMON /EE/ FUEL
      COMMON /FLOOD/ MACRO1
      COMMON /FLOOD1/ A,S,KPOINT,X
C
C
C*****************************************************************
C*                                                               *
C*    THIS SUBROUTINE IS THE EXECUTIVE PROGRAM AFTER MIXING HAS CEASED *
C*    FOR THE FIRST ORDER IMPLICIT INTEGRATION ROUTINE.  IT IS MAINLY  *
C*    CONCERNED WITH SELECTING THE INITIAL CONDITIONS FOR THE          *
C*    ITERATIVE SCHEME AND CHOOSING THE PROPER STEP SIZE.              *
C*                                                               *
C*****************************************************************
C
C
      KPRINT=0
      YNOEQ = 0.
      IF (MACRC .GE. 1) TW=0.
C
C          CALL OUTONE TO PRINT HEADINGS
C
      IF(MACRO .GT.0)GO TO 138
      IF(MACRO1.GT.0)GO TO 138
      IF(NSPRAY.NE.0)GO TO 138
      CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,1,YNOEQ)
      CALL OUTCNE(NIND,NDEP,X,GO,YO,XZO,YNOO,TO,2,YNOEQ)
  138 ACCUR=1.E-4
      IF (MACRO1 .GE. 1) XPRINT=XPRINT+2*DELTAX
```

```
FORTRAN IV G LEVEL  20                 INTGRT                                                    PAGE 0002
 0032              MAXITR=50
 0033              KSTOP=0
 0034              XPRINT=X0
 0035              STEP=DELTAX
 0036              IF (MACRO .GE. 1) GO TO 140
 0037              IF (MACRO1 .EQ. 1) GO TO 140
 0038              X=X0
             C
             C*****WHEN FUEL IS LIQUID OR SOLID WE MUST COMPUTE
             C     THE AMOUNT EVAPORATED OR GASIFIED.
 0039              IF(NSPRAY.EQ.0)GO TO 140
 0040              IF(SS.NE.0.)GO TO 140
 0041              A=AREA(1)
             C
             C*********SUBROUTINE SPRAY COMPUTES THE AMOUNT OF LIQUID
             C         OR SOLID FUEL VAPORIZED OR GASIFIED
             C
 0042              CALL SPRAY(A,STEP,RATES,NT,NSPRAY,TB,TO,P,GO)
             C
             C*********PROCEED TO CALCULATE A NEW COMPOSITION AND
             C         TEMPERATURE BY MIXING THE GAS STREAM WITH
             C         THE EVAPORATED FUEL.--THESE COMPUTATIONS
             C         ARE PERFORMED BY SUBROUTINE UPDATE.
             C
 0043              CALL UPDATE(GO,TO,XZO,YNOO,YO,RATES,TB,G2,T2,XZ2,Y2,YNO2,NIND,
                  1          NDEP,NCCMP,CPAVG,CPCOEF,NSPRAY,ICODE,SS)
 0044              CALL THERMO(T2,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
             C
             C         CALCULATE ADIABATIC FLAME TEMPERATURE FOR ALL THE FUEL
             C
 0045              G3=GO + FUEL
 0046              NTOTAL=NIND+NDEP
 0047              DO 49 I=1,NTOTAL
 0048              IF (ICODE(I) .EQ. 1) GO TO 47
 0049              IF (I .GT. NIND) GO TO 46
 0050              YTEMP(I)=GO*YO(I)/G3
 0051              GO TO 49
 0052           46 II = I-NIND
 0053              XZTEMP(II)=GO*XZO(II)/G3
 0054              GO TO 49
 0055           47 IF (I .GT. NIND) GO TO 48
 0056              YTEMP(I)=FUEL/G3
 0057              GO TO 49
 0058           48 II = I-NIND
 0059              XZTEMP(II) = FUEL/G3
 0060           49 CONTINUE
 0061              CALL TADB(NIND,NDEP,NCOMP,YTEMP,XZTEMP,Y,XZ,DELH,DELALP,
                  1  B,GAMMA,CPCOEF,CPAVG,G3,G,T2,TADAB,HEAT)
 0062              PRINT 499,TADAB
 0063          499 FORMAT(1H1,58X,'COMBUSTION/POLUTION MODEL',//64X,'OUTPUT',
                 1       ' SUMMARY',//57X,19('*'),////T20,'ADIABATIC FLAME ',
                 2       'TEMPERATURE OF VAPORIZED LIQUID/SOLID FUEL = ',F10.2,' K',
                 3       /)
```

```
FORTRAN IV G LEVEL  20                  INTGRT
      C                                                                                       PAGE 0003
      C         CALL OUTONE TO PRINT HEADINGS
      C
              TO=T2
              CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,1,YNOEQ)
              CALL OUTONE(NIND,NDEP,X,GO,YO,XZO,YNOO,TO,2,YNOEQ)
      C
      C
      C---------RE-INITIALIZE
      C
      C
              DO 118 I=1,NIND
          118 YO(I)=Y2(I)
              DO 119 I=1,NDEP
          119 XZO(I)=XZ2(I)
              YNOO=YNO2
              TO=T2
              GO=G2
          140 G=GO
              T=TO
              YNO=YNOO
              YNOEQ=0.
              DO 1 II = 1,NIND
              YO(II) = YO(II)
              VOLD(II)= YO(II)
            1 Y(III) = YO(II)
              DO 2 II = 1,NDEP
              XZOLD(II) = XZO(II)
            2 XZ(II) = XZO(II)
              IF(NSPRAY.NE.0)GO TO 142
              IF (MACRO1 .GE. 1) GO TO 142
              IF (MACRO .NE. 0) GO TO 142
              CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,2,YNOEQ)
          142 KOUNT=0
              TOLD= TO
              GOLD= GO
              YNOLD= YNOO
              KOOK=0
              IF (MACRO .NE. 3) GO TO 1421
              STEP=DELTAX
              HTC(1)=0.
              HTC(2)=0.
              HTC(3)=0.
              QTRAN=0.
              TS=TO
              TCOMB = TO
              T = TO
         1421 XOLD=XO
              IF (MACRO .EQ. 2) GO TO 62
              IF (MACRO1 .EQ. 1) GO TO 52
              IF(NSPRAY.NE.0)GO TO 311
      C
      C       IF SPRAY IS LIQUID OR SOLID GO TO 311
```

```
                C      TO CHECK FOR FUEL AVAILABILITY.
                C
                C
                C**** CHECK FOR OXYGEN AVAILABILITY
                C
                C
                C      ASSUME,AS AN INITIAL GUESS IN THE NEWTON-RAPHSCN,
                C      THAT 50 PERCENT OF OXYGEN REACTS WITH THE FUEL.
                C
 0107                  Y(1) = .5*YO(1)
                C
                C          CALCULATE THE NUMBER OF MOLES OF O2 CONSUMED,Y1R1,
                C          IF ALL THE FUEL BURNS TO CO .
                C
 0108                  Y1R1= (B(1,1)/GAMMA(1,1))*XZO(1)
                C
                C          CHECK IF ENOUGH OXYGEN IS AVAILABLE TO BURN
                C          ALL THE FUEL
                C
 0109                  IF(YO(1).GT.Y1R1) GO TO 300
 0110                  Y2ADD=-.00001
 0111                  GO TO 310
                C
                C      IF THERE IS ENOUGH OXYGEN TO AT LEAST BURN
                C      FUEL TO CO, CHECK HOW MUCH OF THE CO CAN BE
                C      BURNED TO CO2 WITH REMAINING OXYGEN.
                C
                C      XZ2R1=NUMBER OF MOLES OF CO PRODUCED PER MOLE OF FEED
                C      XZO(2)=MOLE FRACTION OF CO
                C      GAMMA(2,1)=STCCHICMETRIC COEFFICIENT OF CO IN REACTION 1.
                C      GAMMA(1,1)=STOCHIOMETRIC COEFFICIENT OF FUEL IN REACTION 1.
                C      XZO(1)=MOLE FRACTION OF GASEOUS FUEL IN THE FEED
                C      B(1,2)=STOCHIOMETRIC COEFFICIENT OF OXYGEN IN REACTION 2.
                C
                C      REACTION 1=  FUEL + OXYGEN= CO + H2O
                C      REACTION 2=  CO + OXYGEN= CO2
                C
 0112             300 XZ2R1=XZO(2)-(GAMMA(2,1)/GAMMA(1,1))*XZO(1)
                C
                C      XZ2R1=NUMBER OF MOLES CO AVAILABLE FROM REACTION 1
                C            PLUS THAT INITIALLY PRESENT IN THE INLET GAS.
                C
                C      Y1R2=MOLES OF O2 CONSUMED BY OXIDATION OF CO.
                C
 0113                  Y1R2=(B(1,2)/GAMMA(2,2))*XZ2R1
                C
                C      IF THE OXYGEN AVAILABLE IS NOT SUFFICIENT TO
                C      BURN ALL THE CO TO CO2,GO TO 320 AND COMPUTE
                C      HOW MUCH CO2 CAN BE PRODUCED WITH O2 THAT'S LEFT.
                C
 0114                  IF(YO(1).LT.(Y1R1+Y1R2)) GO TO 320
                C
 0115                  Y2ADD=(GAMMA(2,1)/GAMMA(1,1))*XZO(1)
```

```
              C      Y2ADD=MOLES OF CO  THAT CAN BE OXIDIZED TO CO2
              C            IF THERE IS ENOUGH OXYGEN TO BURN ALL THE
              C            FUEL TO CO2.
              C
 0116                GO TO 310
              C
 0117           320 Y2ADD=(B(2,2)/B(1,2))*(YO(1)-Y1R1)
              C
              C            THE ABOVE CALCULATION REFLECTS THAT
              C            ONLY A PORTION OF THE CO CAN BE BURNED
              C            TO CO2 FOR LACK OF OXYGEN.
              C
 0118           310 Y(2)=YO(2)-0.49990*Y2ADD
 0119                GO TO 325
              C
              C
              C**** CHECK FOR GAS-FUEL AVAILABILITY IF FUEL IS
              C      INJECTED IN THE LIQUID OR SOLID STATE.
              C
              C          COMPUTE THE AMOUNT OF CO THAT CAN BE PRODUCED.
              C          WITH AVAILABLE GASEOUS FUEL.
              C
 0120           311 Y1R1=B(1,1)/GAMMA(1,1)*XZO(1)
              C
              C      Y1R1=AMOUNT OF OXYGEN CONSUMED BY OXIDATION
              C           OF AVAILABLE FUEL TO CO.
              C
              C      IF THERE IS ENOUGH OXYGEN TO BURN TO CO,PROCEED
              C      TO CALCULATE HOW MUCH CO CAN BE BURNED TO CO2
 0121                IF(YO(1).GT.Y1R1)GO TO 312
              C
              C
              C      IF THERE IS NOT ENOUGH OXYGEN TO PRODUCE CO2
              C      I WANT AT LEAST TO PRODUCE A TINY FRACTION OF IT.
 0122                Y2ADD=-0.00001
 0123                GO TO 324
              C
              C          COMPUTE THE AMOUNT OF CO PRODUCED IF
              C          REACTION 1 GOES TO COMPLETION AND ADD
              C          TO CO ENTERING WITH THE FUEL.
              C
 0124           312 XZ2R1=XZO(2)- GAMMA(2,1)/GAMMA(1,1)*XZO(1)
              C
              C      Y1R2=AMOUNT OF OXYGEN CONSUMED BY REACTION 2
              C
 0125                Y1R2=(B(1,2)/GAMMA(2,2))*XZ2R1
 0126                IF(YO(1).LT.(Y1R1+Y1R2))GO TO 313
 0127                Y2ADD=GAMMA(2,1)/GAMMA(1,1)*XZO(1)
 0128                GO TO 324
 0129           313 Y2ADD=(B(2,2)/B(1,2))*(YO(1)-Y1R1)
 0130           324 Y(2)=YO(2)-0.49990*Y2ADD
 0131                Y(1)=YO(1)-0.5*(Y1R1+Y1R2)
 0132                Y(1)=YO(1)*0.5
```

```
  325 KOOK=0
      IF (MACRO .EQ. 3) GO TO 326
      T=TADAB*0.93
      IF(NSPRAY.GT.0)T=2000.
  326 TTO = T
      IF (MACRO .GE. 1) GO TO 52
   51 IF (DELTAX.EQ.0.0) DELTAX = (XFINAL-XO)/128.
      IF(PINT.LT.DELTAX) DELTAX=PINT
      XPRINT = XPRINT + PINT
   52 IF (KODE(2).NE.2)                        GO TO 330
      IF (MACRO .EQ. 3) GO TO 63
      KODE(1) = 2
      KODE(2)=0
      DELTX = DELTAX
      XPRINT =XO+DELTAX
      DO 65 II= 1,3
   65 HTC(II) = 0.0
      IF (MACRO .GE. 1) GO TO 62
      GO TO 330
C
C
C******* CALCULATE THE NEXT PRINT POSITION.
C
C
    9 IF((XFINAL-XPRINT) .GT. (PINT +DELTAX)) GO TO 3
      XPRINT = XFINAL
      KSTOP =  1
      GO TO 4
    3 XPRINT = XPRINT + PINT
C
C
C
C
C**** GET READY TO TAKE ANOTHER INTEGRATION STEP
C
C
C
    4 IF(NSPRAY.EQ.0)GO TO 44
      CALL SPRAY(A,STEP,RATES,NT,NSPRAY,TB,T,P,G)
C
      CALL UPDATE(G,T,XZ,YNC,Y,RATES,TB,G2,T2,XZ2,Y2,YNO2,NIND,
     1              NDEP,NCOMP,CPAVG,CPCOEF,NSPRAY,ICODE,SS)
C
      DO 41 I=1,NIND
      YO(I)=Y2(I)
   41 YO(I)=Y2(I)
      DO 42 I=1,NDEP
      XZO(I)=XZ2(I)
   42 XZ(I)=XZ2(I)
      YNOO=YNO2
      YNO=YNO2
      TO=T2
      T=T2
```

```
            G=G2
            GO=G2
         44 DO 5 II=1,NIND
            YOLD(II) = YO(II)
          5 Y(II) = YO(II)
            DO 22 II = 1,NDEP
         22 XZOLD(II) = XZ(II)
         23 XOLD = X
            TOLD = T
            GOLD = G
            YNOLD = YNO
      C******* CHOOSE THE NEXT INTEGRATION STEP LENGTH.
      C
      C     AT EVERY NEW INTEGRATION STEP MACRO1=0 THE FIRST TIME THROUGH,
      C     THEN IT REVERTS TO MACRO1=1
      C
        330 IF (MACRO .GE. 1) GO TO 62
            IF((XPRINT-XOLD).GE. (2.*DELTAX))  GO TO 6
            IF((XPRINT-XOLD).LE.(1.0001*DELTAX   )) GO TO 7
            STEP = .5*(XPRINT - XOLD)
            GO TO 8
          6 STEP = DELTAX
            GO TO 8
          7 STEP = XPRINT - XOLD
            KPRINT = 1
          8 X = XOLD + STEP
            KPOINT=1
            GO TO 21
         20 KPOINT = KPOINT + 1
            KO = KPOINT-1
         21 IF( X.GT.XPOINT(KPOINT)) GO TO 20
            THTA=(X - XPOINT(KO))/(XPOINT(KPOINT) - XPOINT(KO))
            A = AREA(KO)+ THTA*(AREA(KPOINT) - AREA(KO))
            S = PERIM(KO)+ THTA*(PERIM(KPOINT) -PERIM(KO))
            IF(KODE(1) .LE. 0) GO TO 60
            TW = TWALL(KO) + THTA*(TWALL(KPOINT)-TWALL(KO))
            GO TO 62
         60 IF(KODE(2) .LE. 0) GO TO 61
            IF(KODE(2).EQ.2) GO TO 63
            TS = TSPEC(KO) + THTA*(TSPEC(KPOINT) - TSPEC(KO))
            GO TO 62
         63 CALL QUENCH(TCOMB,X,XOLD,GOLD,P,A,QNCHRT,QNCHTP,TS)
            TCOMB = TS
            GO TO 62
         61 QTRAN = QSPEC(KO) + THTA*(QSPEC(KPOINT) - QSPEC(KO))
         62 CONTINUE
      C******* CALL 'SOLVE' THE SUBROUTINE WHICH SOLVES ,VIA. A NEWTON -
      C        RAPHSON METHOD- THE SET OF NONLINEAR ALGEBRAIC EQUATIONS
      C        RESULTING FROM THE FIRST ORDER IMPLICIT  FINITE DIFFERENCE
      C        SCHEME USED TO INTEGRATE THE DIFFERENTIAL  EQUATIONS
             CALL      SOLVE(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
           1                   YO,TTO,GAMMA,XZOLD,
           2                   XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
     3                 DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
     4                 MMINV,XZ,AJACOB,FUN,KODE,GO,G,P,T,TOLD,TW,TS,
     5                 QTRAN,A,S,STEP,ACCUR,Y1MIN,MAXITR,KCESS,NOPT,
     6                 IBOMB,NSPRAY)
      IF(IBOMB.NE.0) RETURN
      IF(KCESS .LT. 0) GO TO 111
      IF (MACRO .GE. 1) RETURN
      CALL POLUT(P,T,GOLD,G,YNOLD,STEP,A,XZ(4),Y(1),YNO,YNOEQ,SS,MACRO)
      SS=SS+STEP
  100 IF(KPRINT .GT. 0) GO TO 50
      IF(KODE(1).NE.2) GO TO 4
      IF(T.LT.(0.95*TADAB).AND.ABS(T-TOLD).GT.0.1) GO TO 4
      XPRINT=X
      GO TO 50
   50 CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,2,YNOEQ)
      IF(X.GE.XFINAL)RETURN
      IF(KSTOP .GT. 0) GO TO 500
      KPRINT = 0
      IF ( KODE(1).NE.2) GO TO 9
      IF(T.LT.(0.95*TADAB).AND.ABS(T-TOLD).GT.0.1) GO TO 9
      KODE(1) = 0
      KODE(2) = 2
      DELTAX = DELTX
      TCOMB = T
      GO TO 9
  111 WRITE(6,1001)
 1001 FORMAT(1H1,'THE NEWTON-RAPHSON ITERATION IN SOLVE HAS FAILED TO
     1CONVERGE.  CURRENT VALUES OF INTEREST ARE AS FOLLOWS.')
      CALL OUTONE(NIND,NDEP,X,G,Y,XZ,ANOX,T,2,YNOEQ)
      IBOMB=1
  500 RETURN
 1010 CONTINUE
 1011 CONTINUE
      IBOMB=1
      RETURN
      END
```

```
                                                                                        PAGE 0001
FORTRAN IV G LEVEL  19                  JACOB
 0001               SUBROUTINE JACOB(NIND,NDEP,NDIM,NCOMP,DABINV,YO,Y,GAMBIV,B,XZO,
                   1                    YO,TTC,GAMMA,XZOLD,STEP,
                   2                    DELALP,CPCOEF,DCOF, DGIDY,DXZDY,R,DRDY,DRDXZ,
                   3                    DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,XZ,
                   4                    AJACOB,FUN,KODE,GO,P,T,TW,TS,QTRAN,A,S,G,NOPT,
                   5 IBCMB)
 0002               DIMENSION DABINV(NIND),YO(NIND),Y(NIND),GAMBIV(NDEP,NIND)
 0003               DIMENSION B(NIND,NIND), XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
 0004               DIMENSION DCOF(NIND,14),YO(NIND),GAMMA(NDEP,NIND),XZOLD(NDEP)
 0005               DIMENSION DGIDY(NIND),DXZDY(NDEP,NIND),R(NIND),DRDY(NIND,NIND)
 0006               DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
 0007               DIMENSION DGCPDY(NIND),DELH(NIND),DHDT(NIND)
 0008               DIMENSION XZ(NDEP),AJACOB(NDIM,NDIM),FUN(NDIM)
 0009               DIMENSION KODE(NOPT)
 0010               DIMENSION HTC(3),   RCON(10)
 0011               MAXTIM = 100
 0012               MAX = 0
 0013            28 MAX = MAX + 1
 0014               IF(MAX .GT. MAXTIM) GO TO 30
              C
              C ***    CALCULATE THE TOTAL MOLAR FLOW RATE OF GAS,G,AND THE DERIVATIVE
              C        W.R.T. THE INDEPENDENT COMPOSITION VARIABLES.
              C
 0015               ANUM = 1.
 0016               DENOM=1.
 0017               DO 1 KK =1,NIND
 0018               ANUM= ANUM - DABINV(KK)*YO(KK)
 0019             1 DENOM = DENOM - DABINV(KK)*Y(KK)
 0020               G = GO*ANUM/DENOM
              C
              C
              C******** CALCULATE THE PARTIAL OF  1./G  W.R.T. THE INDE-
              C      PENDENT COMPONENTS Y(I).  THIS IS STORED IN DGIDY.
              C
              C
 0021               DO 2 KK = 1,NIND
 0022             2 DGIDY(KK) = - DABINV(KK)/(GO*ANUM)
              C
              C***  CALCULATE THE DEPENDENT COMPOSITIONS AND THEIR DERIVATIVES W.R.T.
              C      THE INDEPENDENT COMPOSITIONS.
              C
 0023               GOBYG = GO/G
 0024               DO 4 KK = 1,NDEP
 0025               T1 = 0.
 0026               T2 = 0.
              C
              C******** CALCULATE THE CONCENTRATIONS OF THE DEPENDENT COMPONENTS
              C
 0027               DO 3 JJ = 1,NIND
 0028               T1 = T1 + GAMBIV(KK,JJ)*Y(JJ)
 0029             3 T2 = T2 + GAMBIV(KK,JJ)*YO(JJ)
 0030               XZ(KK) = GOBYG*(XZO(KK)-T2) + T1
              C
```

```
      C******** CALCULATE THE PARTIAL OF XZ,DXZDY,W.R.T. Y .
      C
            DO 4 LL=1,NIND
          4 DXZDY(KK,LL)=DGIDY(LL)*GO*XZO(KK)+GAMBIV(KK,LL)- DGIDY(LL)*GO*T2
            DO 25 KK = 1,NDEP
      C
      C          CHECK FOR NEGATIVE VALUES OF XZ(DEPENDENT COMPONENTS)
      C
            IF(XZ(KK).LE.0.C) GO TC 26
         25 CONTINUE
            GO TO 30
         26 AMU = 0.5
            DO 27 KK = 1,NIND
         27 Y(KK) = (1.-AMU)*YO(KK) + AMU*Y(KK)
            GO TO 28
         30 IF((XZ(1) .GT. .0001) .AND. (XZ(2) .GT. .0001))GO TO 31
            A1= RCON(1)
            E1= RCON(2)
            C11=RCON(3)
            C12=RCON(4)
            C13=RCON(5)
            C10 = C11+C12+C13
            CA= P/(14.7*.C8205)
            A1 = A1*28.32*(CA**C10)
            CA1= EXP(-E1/(1.987*T))
            C1= A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(3)**C13)
            IF(XZOLD(1).LT.1.E-40) GO TO 33
            IF(XZ(1) .GT. .0001) GC TO 34
            XZ1S=XZ(1)
            XZ(1) = -((G*XZOLD(1))/(A*GAMMA(1,1)*STEP))/C1
            IF(XZ(1).LE.1.E-9)XZ(1)=1.E-9
            XZ(1) = XZ(1)**(1./C12)
            IF(XZ1S.LT.XZ(1).AND.XZ1S.GT.0.0) XZ(1)=XZ1S
            GO TO 34
         33 XZ(1) = XZCLD(1)
         34 IF(XZOLD(2).LT.1.E-40.AND.XZOLD(2).NE.0.0) GO TO 35
            IF(XZ(2) .GT. .0001) GO TO 31
            A2=RCON(6)
            E2=RCON(7)
            C21=RCON(8)
            C22=RCON(9)
            C23=RCON(1C)
            C20=C21+C22+C23
            A2 =A2*28.32*(CA**C20)
            CA2=EXP(-E2/(1.987*T))
            C2=A2*CA2*( (1./T)**C20)*(Y(1)**C21)*(XZ(3)**C23)
            R(1)= C1*(XZ(1)**C12)
            XZ2S=XZ(2)
            XZ(2) =-((G*XZCLD(2))/(A*STEP) + GAMMA(2,1)*R(1))/(GAMMA(2,2)*C2)
            XZ(2) =  XZ(2)**(1./C22)
            IF(XZ2S.LT.XZ(2).AND.XZ2S.GT.0.0) XZ(2)=XZ2S
            GO TO 31
         35 XZ(2) = XZCLD(2)
```

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FORTRAN IV G LEVEL  19                JACOB                                                    PAGE 0003
            C********CALCULATE THE FUNCTIONS ON THE RIGHT HAND SIDE OF THE NDIM
            C         DIFFERENTIAL EQUATIONS AND ALSO THE JACOBIAN MATRIX
            C         CORRESPONDING TO THESE FUNCTIONS.
 0079          31 CONTINUE
            C
            C
            C******** CALL SUBROUTINE RATE TO CALCULATE DRDXZ AND DRDT
            C          WHICH ARE THE DERIVATIVES OF THE SPECIFIC REACTION
            C          VELOCITY, OF EACH OF THE COMBUSTION REACTIONS,
            C          WITH RESPECT TO XZ AND T.
            C
            C
 0080             CALL       RATE(NIND,NDEP,Y,XZ,P,T,RCON,R,DRDY,DRDXZ,DRDT)
            C
            C******** CALCULATE DRDY WHICH IS THE DERIVATIVE OF THE SPE-
            C          CIFIC REACTION VELOCITY WITH RESPECT TO Y.
            C
 0081             DO 6 II = 1,NIND
 0082             DO 6 JJ = 1,NIND
 0083             T1 = 0.
 0084             DO 5 KK = 1,NDEP
 0085           5 T1 = T1 + DRDXZ(II,KK)*DXZDY(KK,JJ)
 0086           6 DRDY(II,JJ) =  DRDY(II,JJ)+T1
 0087             DO 7 II = 1,NDIM
 0088             DO 7 JJ = 1,NDIM
 0089           7 AJACOB(II,JJ) = 0.
 0090             T0 = 0.
 0091             DO 8 II = 1,NIND
            C
            C      THE FOLLOWING STATEMENTS DOWN TO AND INCLUDING STATEMENT 12
            C        CALCULATE THE FIRST NIND FUNCTIONS AND THE PARTIAL DERIVATIVES
            C        OF THESE FUNCTIONS W.R.T. THE INDEPENDENT COMPOSITION VARIABLES
            C        AND THE TEMPERATURE.
            C
 0092           8 T0 = T0 - DELALP(II)*R(II)
 0093             T0 = A*T0/G
 0094             DO 12 LL = 1,NIND
 0095             T1 = 0.
 0096             T2 = 0.
 0097             DO 10 JJ = 1,NIND
 0098             C1 = B(LL,JJ) - Y(LL)*DELALP(JJ)
 0099             T1 = T1+ C1*R(JJ)
 0100             T2 = T2 + C1*DRDT(JJ)
 0101             DO 10 MM = 1,NIND
 0102          10 AJACOB(LL,MM) = AJACOB(LL,MM) + C1*DRDY(JJ,MM)
 0103             DO 11 MM = 1,NIND
 0104             AJACOB(LL,MM) = A*AJACOB(LL,MM)/G + A*DGIDY(MM)*T1
 0105             IF(MM.EQ.LL) AJACOB(LL,MM) = AJACOB(LL,MM)+T0
 0106          11 CONTINUE
 0107             AJACOB(LL,NDIM) = A*T2/G
 0108          12 FUN(LL) = A*T1/G
 0109             IF(KODE(2) .GT. 0)GO TO  21
          C
```

```
      C********CALCULATE THE FUNCTION CN THE R.H.S. OF THE TEMP. D.E. AND
      C        THE PARTIAL DERIVATIVES OF THIS FUNCTION W.R.T. THE INDEPENDENT
      C        COMPOSITICN VARIABLES AND TEMPERATURE.
      C
            CALL       THERMO(T,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
        990 CONTINUE
            T1=0.
            T2=C.
            T3=0.
            DO 13 LL = 1,NIND
            T1 = T1 + Y(LL)*CP(LL)
         13 T2 = T2 + Y(LL)*DCPDT(LL)
            DO 14 LL = 1, NDEP
            LPNIND = LL + NIND
            T1 = T1+XZ(LL)*CP(LPNIND)
         14 T2 = T2+XZ(LL)*DCPDT(LFNIND)
            DO 16 LL = 1,NIND
            DGCPDY(LL) = CP(LL)
            DO 15 KK=1,NDEP
            KPNIND = KK + NIND
         15 DGCPDY(LL) = CGCPDY(LL) + CP(KPNIND)*DXZCY(KK,LL)
         16 DGCPDY(LL) = (-DGCPDY(LL)/(G*T1) + DGIDY(LL))/T1
            DGCPDT = - T2/(G*T1*T1)
            DO 17 JJ = 1, NIND
         17 T3 = T3 -DELH(JJ)*R(JJ)
            CALL       HLCSS(T,TW,QTRAN,HTC,QLCSS,DQLDT,KODE,NOPT)
            T3 = A*T3-S*QLOSS
            FUN(NDIM) = T3/(G*T1)
            DO 19 KK = 1,NIND
            AJACOB(NDIM,KK) = 0.
            DO 18 JJ = 1,NIND
         18 AJACOB(NDIM,KK) = AJACOB(NDIM,KK) - DELH(JJ)*DRDY(JJ,KK)
         19 AJACOB(NDIM,KK) = AJACCB(NDIM,KK) * A/(G*T1) + DGCPDY(KK)*T3
            DO 20 JJ = 1,NIND
         20 AJACOB(NDIM,NDIM) = AJACOB(NDIM,NDIM) - DELH(JJ)*DRDT(JJ)-DHDT(JJ)
           1*R(JJ)
            AJACOB(NDIM,NDIM)=(AJACOB(NDIM,NDIM)*A - S*DQLDT)/(G*T1) + DGCPDT
           1*T3
       9990 CONTINUE
            RETURN
         21 DO 22 LL = 1,NDIM
         22 AJACOB(NDIM,LL) = 0.
            RETURN
       1000 WRITE(6,1001)
       1001 FORMAT(1H ,'A FEASIBLE SOLUTION CANNOT BE FOUND....JACOB')
            IBOMB=1
            RETURN
            END
```

```
FORTRAN IV G LEVEL  20                  SOLVE                                                PAGE 0001
 0001              SUBROUTINE SOLVE(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
                  1                  YO,TTO,GAMMA,XZOLD,
                  2                  XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
                  3                  DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
                  4                  MMINV,XZ,AJACOB,FUN,KODE,GO,G,P,T,TOLD,TW,TS,
                  5                  QTRAN,A,S,STEP,ACCUR,Y1MIN,MAXITR,KCESS,NOPT,
                  6                 IBOMB,NSPRAY)
 0002              DIMENSION DABINV(NIND),YO(NIND),Y(NIND),YOLD(NIND),YO(NIND)
 0003              DIMENSION GAMBIV(NDEP,NIND),GAMMA(NDEP,NIND),XZOLD(NDEP)
 0004              DIMENSION B(NIND,NIND), XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
 0005              DIMENSION DCOF(NIND,14)
 0006              DIMENSION DGIDY(NIND),DXZDY(NDEP,NIND),R(NIND),DRDY(NIND,NIND)
 0007              DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
 0008              DIMENSION DGCPDY(NIND),DELH(NIND),DHDT(NIND),LMINV(NDIM)
 0009              DIMENSION MMINV(NDIM)
 0010              DIMENSION XZ(NDEP),AJACOB(NDIM,NDIM),FUN(NDIM)
 0011              DIMENSION HTC(3),   RCON(10)
 0012              DIMENSION KODE(NOPT)
 0013              DIMENSION YSAVE(2)
            C
            C*************************************************************
            C*                                                          *
            C*    THIS SUBROUTINE SETS UP AND SOLVES BY NEWTON-RAPHSON THE   *
            C*    EQUATIONS FOR THE FIRST ORDER IMPLICIT FINITE DIFFERENCE   *
            C*    SCHEME. IT USES SUBROUTINE JACOB TO COMPUTE THE JACOBIAN.  *
            C*                                                          *
            C*************************************************************
            C
            C
 0014              IDBUG=1
 0015              ITER=0
            C
            C
            C          IF GAS TEMPERATURE PROFILE IS NOT SPECIFIED GO TO 30
            C
 0016              IF(KODE(2).LE.0)GO TO 30
 0017              T=TS
 0018              TTO=T
 0019           30 CONTINUE
 0020          100 ITER=ITER + 1
 0021              IF(ITER.GT.MAXITR) GO TO 300
 0022              DO 50 KK=1,NIND
 0023           50 YSAVE(KK)=Y(KK)
 0024              CALL        JACOB(NIND,NDEP,NDIM,NCOMP,DABINV,YO,Y,GAMBIV,B,XZO,
                1                    YO,TTO,GAMMA,XZOLD,STEP,
                2          DELALP,CPCOEF,DCOF ,DGIDY,DXZDY,R,DRDY,DRDXZ,
                3                    DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,XZ,
                4                    AJACOB,FUN,KODE,GO,P,T,TW,TS,QTRAN,A,S,G,NOPT,
                5 IBOMB)
 0025              IF(IBOMB.NE.0) RETURN
 0026              ICONV=0
 0027              DO 51 KK=1,NIND
 0028              IF(Y(KK).EQ.YSAVE(KK).OR.ABS((Y(KK)-YO(KK))/YO(KK)).GE..001.OR.
                                                                                  PAGE 0002
FORTRAN IV G LEVEL  20                    SOLVE
                 1 ITER.EQ.1) GO TO 52
 0029          51 CONTINUE
 0030             ICONV=1
 0031          52 CONTINUE
            C
            C-------- AS CONVERGENCE IS ACHIEVED FUN(NDIM) APPROACHES ZERO
            C
 0032             DO 1 II=1,NIND
 0033           1 FUN(II)= Y(II)-STEP*FUN(II)- YOLD(II)
 0034             IF(KODE(2) .GT. 0) GO TO 6
            C
            C-------- IF KODE(2) = 1, GAS TEMPERATURE PROFILE IS SPECIFIED.
            C
 0035             FUN(NDIM)= T  -STEP*FUN(NDIM)-TOLD
 0036             GO TO 7
            C
            C          WHEN GAS TEMPERATURE PROFILE IS SPECIFIED,
            C          FUN(NDIM) BECOMES ZERO SINCE T=TS.
            C
 0037           6 FUN(NDIM)=T-TS
 0038           7 CONTINUE
            C
            C
            C********AFTER THE CALL TO JACOB, THE MATRIX AJACOB CONTAINS THE
            C         PARTIAL DERIVATIVES OF FUN W.R.T. THE INDEPENDENT COMPOSITION
            C         VARIABLES.  THE FOLLOWING STATEMENTS DOWN TO AND INCLUDING
            C         STATEMENT 3 CALCULATE THE JACOBIAN CORRESPONDING TO THE FIRST
            C         ORDER IMPLICIT SCHEME USED HERE.
            C
            C
            C
 0039             DO 3 II = 1,NDIM
 0040             DO 3 JJ = 1,NDIM
 0041             AJACOB(II,JJ) = -STEP*AJACOB(II,JJ)
 0042             IF(II.EQ.JJ) AJACOB(II,JJ)= 1. + AJACOB(II,JJ)
 0043           3 CONTINUE
 0044             CALL MINV(AJACOB,NDIM,D,LMINV,MMINV)
 0045             TTO = T
 0046             DO 4 KK = 1,NIND
 0047             YO(KK) = Y(KK)
 0048             IF(KK.EQ.2) GO TO 41
 0049             IF(YOLD(KK).LT.1.E-40) GO TO 43
 0050             IF(Y(KK).LT.1.0E-20) GO TO 4
 0051             GO TO 42
 0052          43 Y(KK)=YOLD(KK)
 0053             GO TO 4
 0054          41 IF(YOLD(KK).GE.1.E-40.OR.YOLD(KK).EQ.0.0) GO TO 42
 0055             GO TO 43
 0056          42 DO 40 JJ=1,NDIM
 0057          40 Y(KK)= Y(KK)- AJACOB(KK,JJ)*FUN(JJ)
 0058           4 CONTINUE
 0059          12 DO 5  JJ = 1,NDIM
 0060           5 T = T- AJACOB(NDIM,JJ)*FUN(JJ)
 0061         130 IF(T.GT.TTO)GO TO 133
```

```
      RATIO=T/TTO
      CHECK=0.95
      IF(RATIO.LT.CHECK)T=TTO*CHECK
         GO TO 134
  133 RATIO=T/TTO
      CHECK=1.05
      IF(RATIO.GT.CHECK) T=TTO*CHECK
  134 IF(Y(1).LE.0..OR.Y(2).LE.0.) GO TO 15
      ADIST = ABS((T-TTO)/100.)
      DO 13 KK = 1,NIND
      HOLD =(ABS (Y(KK) - YO(KK)))/YO(KK)
      IF(HOLD .GT. ADIST) ADIST = HOLD
   13 CONTINUE
      IF(ADIST .LT. .001  ) GO TO 200
      ANORM = 0.
      DO 2 II = 1,NDIM
    2 ANORM = ANORM + FUN(II)*FUN(II)
      ANORM = SQRT(ANORM)
      IF(ANORM .LT. ACCUR) GO TO 200
      IF(ABS((T-TTO)/100.).GE..001) GO TO 15
      IF(ICONV.EQ.0) GO TO 15
      GO TO 200
   15 MAX = 0
   11 MAX = MAX + 1
      IF(MAX .GT. 10) GO TO 20
      IF(Y(1).LE.0.0.OR.Y(2).LE.0.0) GO TO 9
      GO TO 14
    9 AMU = .50
      DO 10 KK = 1,NIND
   10 Y(KK) = (1. - AMU)*YO(KK) + AMU*Y(KK)
      GO TO 11
   14 CONTINUE
      GO TO 100
  200 KCESS = +1
C     T = TTO
C     DO 17 KK = 1,NIND
C  17 Y(KK) = YO(KK)
C     GO TO 400
      RETURN
  300 KCESS = -1
  400 RETURN
   20 WRITE(6,1000)
 1000 FORMAT(1H0,'A FEASIBLE SOLUTION CAN NOT BE FOUND .....SOLVE')
      IBOMB=1
      RETURN
      END
```

```
FORTRAN IV G LEVEL  21                    TADB                                              PAGE 0001

 0001                 SUBROUTINE  TADB(NIND,NDEP,NCOMP,YO,XZO,Y,XZ,DELH,DELALP,B,GAMMA,
                    1                   CPCOEF,CPAVG,GO,G,TO,TADAB,HEAT)
 0002                 DIMENSION YO(NIND),Y(NIND),XZO(NDEP),XZ(NDEP),DELALP(NIND)
 0003                 DIMENSION DELH(NIND),B(NIND,NIND),GAMMA(NDEP,NIND)
 0004                 DIMENSICN CPCOEF(NCOMP,10),CPAVG(NCOMP)
                C 990 CONTINUE
 0005                 IF(YO(1) .GT.  (B(1,1)/GAMMA(1,1))*XZO(1)) GO TO 50
                C     THERE IS  LESS O2 THAN REQUIRED TO CARRY THE FIRST REACTION TO
                C     COMPLETION. CONSIDER THE FIRST REACTION COMPLETELY DOMINATES.
                C     THE HEAT RELEASED IS (IT IS POSITIVE)
 0006                 HEAT =(GO*YO(1))* (DELH(1)/B(1,1))
 0007                 G = GO*(1. - (DELALP(1)/B(1,1))*YO(1))
 0008                 Y(1) = 0.
 0009                 Y(2) =(GO/G)*(YO(2) - B(2,1)/  B(1,1)*YO(1))
 0010                 DO 1 KK = 1,NDEP
 0011               1 XZ(KK) =(GO/G)*(XZO(KK) -  GAMMA(KK,1)/B(1,1)*YO(1))
 0012                 GO TO 100
 0013              50 CONTINUE
                C     THERE IS MORE THAN ENOUGH OXYGEN TO CARRY THE FIRST REACTION TO
                C     COMPLETION.
 0014                 G = GO*(1. - (DELALP(1)/GAMMA(1,1))*XZO(1))
                C     THE HEAT RELEASED BY THE FIRST REACTION GOING TO COMPLETION IS,
 0015                 HEAT =(GO*XZO(1))*DELH(1)/GAMMA(1,1)
 0016                 DO 2 KK = 1,NIND
 0017               2 Y(KK) = (GO/G)*(YO(KK) - B(KK,1)/GAMMA(1,1) * XZO(1))
 0018                 DO 3 KK = 1,NDEP
 0019               3 XZ(KK) = (GO/G)*(XZO(KK) -GAMMA(KK,1)/GAMMA(1,1) *XZO(1))
                C     IS THERE ENOUGH O2 TO COMPLETELY CONVERTE THE CO FORMED BY THE
                C     FIRST REACTION.
 0020                 IF(Y(1) .GT.  B(1,2)/GAMMA(2,2)*XZ(2)) GO TO 75
                C     THERE IS NOT ENOUGH O2 TO TAKE THE SECOND REACTION TO COMPLETION.
                C     THE HEAT RELEASED IS.
 0021                 HEAT = HEAT + G*Y(1)*DELH(2)/B(1,2)
 0022                 G1= G
 0023                 G =G1*(1. - DELALP(2)/B(1,2) *Y(1))
 0024                 Y(2)=(G1/G)*(Y(2) - B(2,2)/B(1,2)*Y(1))
 0025                 DO 4 KK = 1,NDEP
 0026               4 XZ(KK) =(G1/G)*(XZ(KK)- GAMMA(KK,2)/B(1,2)*Y(1))
 0027                 Y(1) = 0.
 0028                 GO TO 100
 0029              75 CONTINUE
                C     THERE IS ENOUGH O2 TO CARRY SECOND REACTION TO COMPLETION.
                C     THE HEAT RELEASED BY THE SECOND REACTION IS.
 0030                 HEAT = HEAT + G*XZ(2)*DELH(2)/GAMMA(2,2)
 0031                 G1= G
 0032                 G =G1*(1. - DELALP(2)/GAMMA(2,2)*XZ(2))
 0033                 DO 5 KK = 1,NIND
 0034               5 Y(KK) =(G1/G)*(Y(KK) - B(KK,2)/GAMMA(2,2) * XZ(2))
 0035                 DO 6 KK = 1,NDEP
 0036                 IF(KK.EQ. 2) GO TO  6
 0037                 XZ(KK) =(G1/G)*(XZ(KK) - GAMMA(KK,2)/GAMMA(2,2) * XZ(2))
 0038               6 CONTINUE
 0039                 XZ(2) = 0.
 0040          100 CONTINUE
                   TL = TO
 0042              TH = 3000.
 0043              FL =-HEAT
 0044              CALL  CAVG(NCOMP,CPCOEF,CPAVG,TO,TH)
 0045              A1= 0.
 0046              DO 11 KK= 1,NIND
 0047           11 A1 = A1+Y(KK)*CPAVG(KK)
 0048              DO 12 KK= 1,NDEP
 0049              KKP= KK+NIND
 0050           12 A1 = A1+XZ(KK)*CPAVG(KKP)
 0051              FH = -HEAT + G*A1*(TH-TO)
 0052              IF(FH .LT. 0.) GO TO 5000
 0053              KOUNT = 0
 0054              TM=0.0
 0055           30 KOUNT =KOUNT +1
 0056              IF(KOUNT .GT.50) GO TO 5001
 0057              TMS=TM
 0058              TM =(TL*FH - TH*FL)/(FH-FL)
 0059              CALL  CAVG(NCOMP,CPCOEF,CPAVG,TO,TM)
 0060              A1 = 0.
 0061              DO 13 KK = 1,NIND
 0062           13 A1 = A1 + Y(KK)*CPAVG(KK)
 0063              DO 14 KK = 1,NDEP
 0064              KKP=KK+NIND
 0065           14 A1 =A1 + XZ(KK)*CPAVG(KKP)
 0066              FM = -HEAT + G*A1*(TM-TO)
 0067              IF(ABS(TM-TMS).LT..01) GO TO 22
 0068              IF(FM .LT. 0.) GO TO 23
 0069              FH = FM
 0070              TH = TM
 0071              GO TO 30
 0072           23 FL =FM
 0073              TL =TM
 0074              GO TO 30
 0075           22 TADAB = TM
             C9990 CONTINUE
 0076              RETURN
 0077         5000 WRITE(6,1111)
 0078         1111 FORMAT(1H0,'THE ADIABATIC FLAME TEMP. IS GT 3000.K')
 0079              TADAB=3100.
 0080              RETURN
 0081         5001 WRITE(6,1112)
 0082         1112 FORMAT(1H ,'THE ADIABATIC FLAME TEMP. WAS NOT LOCATED.')
 0083              TADAB=0.0
 0084              RETURN
             C     DEBUG INIT , TRACE
             C     AT 990
             C     TRACE ON
             C     AT 9990
             C     TRACE OFF
 0085              END
```

```
FORTRAN IV G LEVEL  20                RATE                                          PAGE 0001

 0001             SUBROUTINE RATE(NIND,NDEP,Y,XZ,P,T,RCON,R,DRDY,DRDXZ,DRDT)
 0002             DIMENSION Y(NIND),XZ(NDEP),RCON(10),DRDY(NIND,NIND),R(NIND)
 0003             DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND)
            C***  RATE EXPRESSIONS SUPPLIED BY THE USER ARE OF THE FORM
            C     A. FOR FUEL GOING TO CO AND H2O
            C     R(1)= A1*EXP(-E1/(1.987*T))*((O2)**C11)*((FUEL)**C12)*((H2O)**C13)
            C     B. FOR CO GOING TO CO2.
            C     R(2)= A2*EXP(-E2/(1.987*T))*((O2)**C21)*((CO)**C22)*((H2O)**C23)
            C     THE UNITS HERE ARE,
            C     R , MOLES/(LITER-SEC.)
            C     E1,E2,   CAL./MOLE
            C     T       , DEGREE KELVIN
            C     (COMP.), MOLES/LITER
            C     THE CONSTANTS A1,A2,.....,C23 ARE IN THE ARRAY RCON
 0004             A1 = RCON(1)
 0005             E1 = RCON(2)
 0006             C11= RCON(3)
 0007             C12= RCON(4)
 0008             C13= RCON(5)
 0009             A2 = RCON(6)
 0010             E2 = RCON(7)
 0011             C21= RCON(8)
 0012             C22= RCON(9)
 0013             C23= RCON(10)
 0014             C10 = C11+C12+C13
 0015             C20 = C21+C22+C23
            C     CONVERT THE RATE EXPRESSIONS TO THE UNITS OF MOLES/((CUBIC FT.)*(SEC.))
            C     BY MULTIPLYING BY 28.32 LITERS/CUBIC FOOT. AT THE SAME TIME CONVERT
            C     TO MOLE FRACTIONS.
 0016             CA = P/(14.7*.08205)
 0017             A1 = A1*28.32*(CA**C10)
 0018             A2 = A2*28.32*(CA**C20)
 0019             CA1 = EXP(-E1/(1.987*T))
 0020             CA2 = EXP(-E2/(1.987*T))
 0021             R(1) = A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(1)**C12)*(XZ(3)**C13)
 0022             R(2) = A2*CA2*((1./T)**C20)*(Y(1)**C21)*(XZ(2)**C22)*(XZ(3)**C23)
 0023             DRDY(1,1) = C11*A1*CA1*((1./T)**C10)*(Y(1)**(C11-1.))*(XZ(1)**C12)
                 1            *(XZ(3)**C13)
 0024             DRDY(1,2) = 0.
 0025             DRDY(2,1) = C21*A2*CA2*((1./T)**C20)*(Y(1)**(C21-1.))*(XZ(2)**C22)
                 1            *(XZ(3)**C23)
 0026             DRDY(2,2) = 0.
 0027             DRDXZ(1,1)= C12*A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(1)**(C12-1.))
                 1            *(XZ(3)**C13)
 0028             DRDXZ(1,2)=0.
 0029             DRDXZ(1,3)= C13*A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(1)**C12)
                 1            *(XZ(3)**(C13-1.))
 0030             DRDXZ(1,4)= 0.
 0031             DRDXZ(2,1) =0.
 0032             DRDXZ(2,2)= C22*A2*CA2*((1./T)**C20)*(Y(1)**C21)*(XZ(2)**(C22-1.))
                 1            *(XZ(3)**C23)
 0033             DRDXZ(2,3)= C23*A2*CA2*((1./T)**C20)*(Y(1)**C21)*(XZ(2)**C22)
                 1            *(XZ(3)**(C23-1.))
```

```
FORTRAN IV G LEVEL  20                  RATE                                                        PAGE 0002

 0034              DRDXZ(2,4)= 0.
 0035              DRDT(1) =  R(1)*(E1/(1.987*T*T) - C10/T)
 0036              DRDT(2) =  R(2)*(E2/(1.987*T*T) - C20/T)
 0037              RETURN
 0038              END
```

```
FORTRAN IV G LEVEL  20                  HLOSS                                        PAGE 0001

 0001               SUBROUTINE HLOSS(T,TW,QTRAN,HTC,QLOSS,DQLDT,KODE,NOPT)
 0002               DIMENSION KODE(NOPT)
 0003               DIMENSION HTC(3)
 0004               IF(KODE(3).GT.0) GO TO 1
 0005               QLOSS = HTC(1) + HTC(2)*(T-TW) + HTC(3)*(T**4 - TW**4)
 0006               DQLDT = HTC(2) + 4.*HTC(3)*T**3
 0007               RETURN
 0008             1  QLOSS = QTRAN
 0009               DQLDT = 0.
 0010               RETURN
 0011               END
```

```
FORTRAN IV G LEVEL  20                OUTONE                                                      PAGE 0001

 0001               SUBROUTINE OUTONE(NIND,NDEP,X,G,Y,XZ, YNO,T,KASE,YNOEQ)
 0002               DIMENSION Y(NIND),XZ(NDEP)
 0003               IF(KASE .LT. 2) GO TO 1
 0004               WRITE(6,1000)X,G,T,Y,XZ,YNO,YNOEQ
 0005          1000 FORMAT (1H0,G11.4,10G12.4)
 0006               GO TO 10
 0007             1 WRITE(6,1001)
 0008          1001 FORMAT(//2X,'DISTANCE',4X,'FLOW RATE',7X,'T',10X,'O2',10X,'CO2',
                  1 8X,'FUEL',9X,'CO',10X,'H2O',9X,'N2',10X,'NO',8X,'NO(EQ)',/4X,
                  2 '(FT)',4X,'(G-MOLS/SEC)',5X,'(K)',9X,36('-'),'(MOLE FRACTION)',
                  3 37('-'))
 0009            10 RETURN
 0010               END
```

```
FORTRAN IV G LEVEL  20                CAVG                                    PAGE 0001

               SUBROUTINE CAVG(NCOMP,CPCOEF,CPAVG,T1,T2)
               DIMENSICN CPCOEF(NCOMP,10) , CPAVG(NCOMP)
               DO 10 KK =1,NCCMP
            10 CPAVG(KK) = 0.
               U1= T1/1000.
               H1 = U1
               U2= T2/1000.
               IF(U1.LT. 1.2) GO TO 1
               H2 = U2
               GO TO 50
             1 IF(U2.LE. 1.2) GO TO 2
               H2= 1.2
               GO TO 3
             2 H2 = U2
             3 CONTINUE
               V1=1.
               V2=1.
               DO 4 KK =1,5
               AK= KK
               V1= V1*H1
               V2= V2*H2
               DO 5 KPN = 1,NCCMP
               CPAVG(KPN)= CPAVG(KPN)+CPCOEF(KPN,KK)*(V2 - V1)/AK
             5 CONTINUE
             4 CONTINUE
               IF(U2 .LE. 1.2) GO TO 75
               H2= U2
               H1= 1.2
            50 DO 6 KPN =1,NCOMP
               CPAVG(KPN)= CPAVG(KPN)+CPCOEF(KPN,6)*(H2-H1)+CPCOEF(KPN,7)*ALOG(H
              12/H1)
             6 CONTINUE
               AK = 0.
               V1 = 1.
               V2 = 1.
               DO 7 KK =8,10
               AK= AK+1.
               V1= V1/H1
               V2= V2/H2
               DO 8 KPN =1,NCOMP
               CPAVG(KPN) =CPAVG(KPN) -(1./AK)*CPCOEF(KPN,KK)*(V2 - V1)
             8 CONTINUE
             7 CONTINUE
            75 DO 76 KPN = 1,NCOMP
            76 CPAVG(KPN)=CPAVG(KPN)/(T2 - T1)
               RETURN
               END
```

```
FORTRAN IV G LEVEL  20                CPFIT                                               PAGE 0001
             SUBROUTINE  CPFIT(NPTS,NCON,TO,CPO,TX,CPY,CO,C,FO,F,A,KASE)
             DIMENSION TX(NPTS),CPY(NPTS),C(NCON),FO(NCON),F(NPTS,NCON)
             DIMENSION A(NCON,NCCN)
             DO 25  II = 1,NPTS
             READ(5,2000) TX(II),CPY(II)
             PRINT 125, TX(II), CPY(II)
       125   FORMAT (10X, F10.3, 20X, F10.3)
        25   CONTINUE
      2000   FORMAT(4X,2F10.3)
             TO = TO/1000.
             DO 100 II =1,NPTS
       100   TX(II)= TX(II)/1000.
         1   IF(KASE.GT.0) GO TO 2
             Z= TO
             GO TO 3
         2   Z = 1./TO
         3   FO(1) = Z
             DO 4 II=2,NCON
             IM1 =II-1
         4   FO(II) = FO(IM1)*Z
             DO 5 II = 1,NPTS
             IF(KASE.GT.0) GO TO 6
             Z = TX(II)
             GO TO 7
         6   Z= 1./TX(II)
         7   F(II,1)= Z
             DO 8 KK= 2,NCON
             KKM1 = KK-1
         8   F(II,KK) = F(II,KKM1)*Z
             DO 5 KK= 1,NCON
         5   F(II,KK) = F(II,KK)-FO(KK)
             DO 11 KK = 1,NCCN
             DO 11 II = 1,NCCN
             A(KK,II) = 0.
             DO 11 JJ = 1,NPTS
        11   A(KK,II) = A(KK,II)+ F(JJ,KK)*F(JJ,II)
             DO 12 KK = 1,NCCN
             C(KK)=0.
             DO 12 JJ= 1,NPTS
        12   C(KK)= C(KK)+ F(JJ,KK)*(CPY(JJ)-CPO)
             CALL SIMQ(A,C,NCON,KS)
             IF(KS.LT.1 ) GO TO 15
             WRITE(6,1000)
      1000   FORMAT(' A SINGULAR SET OF EQUATION HAS BEEN ENCOUNTERED')
             GO TO 17
        15   CO = CPO
             DO 16 II = 1,NCCN
        16   CO = CO- C(II)*FO(II)
        17   RETURN
             END
```

```
FORTRAN IV G LEVEL  20                    MIX

 0001              SUBROUTINE MIX(G1,Y1,XZ1,YNO1,T1,G2,Y2,XZ2,YNO2,T2,G3,Y3,XZ3,YNO3,      PAGE 0001
                  1              T3,NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
 0002              DIMENSION Y1(NIND),XZ1(NDEP),Y2(NIND),XZ2(NDEP),Y3(NIND),XZ3(NDEP)
 0003              DIMENSION CPCOEF(NCOMP,10),CPAVG(NCOMP)
             C 990 CONTINUE
             C     DO MATERIAL BALANCES
 0004              G3= G1+G2
 0005              DO 1 KK = 1,NIND
 0006            1 Y3(KK) = (G1*Y1(KK) + G2*Y2(KK))/G3
 0007              DO 2 KK = 1,NDEP
 0008            2 XZ3(KK) = (G1*XZ1(KK) + G2*XZ2(KK))/G3
 0009              YNO3 = (G1*YNO1 + G2*YNO2) / G3
             C     DO ENERGY BALANCE
             C     THE REFERENCE TEMP. IS 298K
 0010              TR=298.
 0011              IF(T1.EQ.T2) GO TO 25
 0012              CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,T1)
 0013              A1 = 0.
 0014              B1 = 0.
 0015              DO 3 KK=1,NIND
 0016              B1 = B1 + Y3(KK)*CPAVG(KK)
 0017            3 A1 = A1 + Y1(KK)*CPAVG(KK)
 0018              DO 4 KK=1,NDEP
 0019              KKP = KK + NIND
 0020              B1 = B1 + XZ3(KK)*CPAVG(KKP)
 0021            4 A1 = A1 + XZ1(KK)*CPAVG(KKP)
 0022              H1 = G1*A1*(T1-TR)
 0023              CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,T2)
 0024              A2 =0.
 0025              B2 =0.
 0026              DO 5 KK=1,NIND
 0027              A2 = A2 + Y2(KK)*CPAVG(KK)
 0028            5 B2 = B2 + Y3(KK)*CPAVG(KK)
 0029              DO 6 KK=1,NDEP
 0030              KKP = KK+NIND
 0031              B2  =B2 + XZ3(KK)*CPAVG(KKP)
 0032            6 A2 = A2 + XZ2(KK)*CPAVG(KKP)
 0033              H2 = G2*A2*(T2-TR)
 0034              F1 = G3*B1*(T1-TR)-H1-H2
 0035              F2 = G3*B2*(T2-TR)-H1-H2
 0036              IF(T1 .GT. T2) GO TO 7
 0037              TL =T1
 0038              FL =F1
 0039              TH =T2
 0040              FH =F2
 0041              GO TO 8
 0042            7 TL=T2
 0043              FL=F2
 0044              TH=T1
 0045              FH=F1
 0046            8 KOUNT =0
 0047              TM=0.0
 0048           99 KOUNT =KOUNT + 1
```

```
FORTRAN IV G LEVEL  20                  MIX                                                    PAGE 0002

 0049              IF(KOUNT.GT.50) GO TO 234
 0050              TMS=TM
 0051              TM = (TL*FH - TH*FL)/(FH-FL)
 0052              AM = 0.
 0053              CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,TM)
 0054              DO 9 KK = 1,NIND
 0055            9 AM = AM + Y3(KK)*CPAVG(KK)
 0056              DO 10 KK =1,NDEP
 0057              KKP = KK+NIND
 0058           10 AM  = AM + XZ3(KK)*CPAVG(KKP)
 0059              FM = G3*AM*(TM-TR)-H1-H2
 0060              IF(ABS(TM-TMS).LT..01) GO TO 100
 0061              IF (FM .LT. 0.) GO TO 11
 0062              FH = FM
 0063              TH = TM
 0064              GO TO 99
 0065           11 FL = FM
 0066              TL = TM
 0067              GO TO 99
 0068          100 T3 = TM
 0069              RETURN
 0070           25 T3 = T1
 0071              RETURN
 0072          234 WRITE(6,1000)
             C9990 CONTINUE
 0073         1000 FORMAT(' A SOLUTION CAN NOT BE FOUND......MIX')
 0074              IBOMB=1
 0075              RETURN
             C     DEBUG INIT,TRACE
             C     AT 990
             C     TRACE ON
             C     AT 9990
             C     TRACE OFF
 0076              END
```

```
FORTRAN IV G LEVEL  20                 THERMO                                               PAGE 0001

0001               SUBROUTINE THERMO(T,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
0002               DIMENSICN CPCOEF(NCOMP,10),DCOF(NIND,14),CP(NCOMP)
0003               DIMENSION DCPDT(NCOMP),DELH(NIND),DHDT(NIND)
0004               TR = T/1000.
0005               IF(T .GT. 1200.) GO TO 100
0006               TR2 = TR *TR
0007               TR3= TR2*TR
0008               TR4= TR3*TR
0009               TR5= TR4*TR
0010               DO 1  II =1,NCOMP
0011               CP(II)=(CPCOEF(II,1) + CPCOEF(II,2)*TR + CPCOEF(II,3)*TR2
                  1        +CPCOEF(II,4)*TR3 + CPCOEF(II,5)*TR4)/1000.
0012             1 DCPDT(II)=(CPCOEF(II,2)+2.*CPCOEF(II,3)*TR +3.*CPCOEF(II,4)*TR2
                  1           +4.*CPCOEF(II,5)*TR3)/(1000.*1000.)
0013               DO 2 II = 1,NIND
0014               DHDT(II)=(DCOF(II,1) +DCOF(II,2)*TR + DCOF(II,3)*TR2
                  1           +DCOF(II,4)*TR3 + DCOF(II,5)*TR4)/1000.
0015             2 DELH(II) =DCOF(II,11)+       (DCOF(II,1)*TR + DCOF(II,2)*TR2/2.
                  1+ DCOF(II,3)*TR3/3. + DCOF(II,4)*TR4/4.  + DCOF(II,5)*TR5/5.
                  2- DCOF(II,13))
0016               RETURN
0017           100 TR1 = 1./TR
0018               TR2 = TR1/TR
0019               TR3 = TR2/TR
0020               TR4 = TR3/TR
0021               DO 4 II = 1,NCOMP
0022               CP(II) =(CPCOEF(II,6) + CPCOEF(II,7)*TR1 + CPCOEF(II,8)*TR2
                  1          + CPCOEF(II,9)*TR3 + CPCOEF(II,10)*TR4)/1000.
0023             4 DCPDT(II) = -(CPCOEF(II,7) + 2.*CPCOEF(II,8)*TR1 + 3.*CPCOEF(II,9)
                  1             *TR2 + 4.*CPCOEF(II,10)*TR3)/(1000.*1000.*TR2)
0024               DO 5 II = 1,NIND
0025               DHDT(II) =(DCOF(II,6) + DCOF(II,7)*TR1 + DCOF(II,8)*TR2
                  1           +DCOF(II,9)*TR3 + DCOF(II,10)*TR4)/1000.
0026             5 DELH(II) = DCOF(II,12) +        ( DCOF(II,6)*TR + DCOF(II,7)*
                  1           ALOG(TR) - DCOF(II,8)*TR1 - DCOF (II,9)*TR2/2.
                  2            - DCOF(II,10)*TR3/3. - DCOF(II,14) )
0027               RETURN
0028               END
```

```
FORTRAN IV G LEVEL  20                BINVER                                        PAGE 0001

 0001              SUBROUTINE BINVER(NIND,B,BINV)
 0002              DIMENSION B(NIND,NIND),BINV(NIND,NIND)
 0003              D = B(1,1)*B(2,2) - B(1,2)*B(2,1)
 0004              BINV(1,1)= B(2,2)/D
 0005              BINV(1,2)= -B(1,2)/D
 0006              BINV(2,1)= -B(2,1)/D
 0007              BINV(2,2)= B(1,1)/D
 0008              RETURN
 0009              END
```

```
FORTRAN IV G LEVEL  20                QUENCH                                              PAGE 0001

            SUBROUTINE QUENCH(TCOMB,X,XOLD,GOLD,P,A,QNCHRT,QNCHTP,TS)
            DIMENSION QNCHRT(3)
            IF(QNCHTP.EQ.1.) GO TO 10
            TRATE=QNCHRT(1)+QNCHRT(2)*TCOMB+QNCHRT(3)*TCOMB*TCOMB
            GO TO 20
         10 TRATE= (QNCHRT(1)+ QNCHRT(2)*TCOMB) * EXP(QNCHRT(3)/TCOMB)
         20 DENS = P/((10.73*1.8/454.) * TCOMB)
            TDROP = TRATE * DENS * A / GOLD
            TS = TCOMB + TDROP * (X-XOLD)
            RETURN
            END
```

```
FORTRAN IV G LEVEL  20                    UPDATE                                                    PAGE 0001

 0001             SUBROUTINE UPDATE(GO,YO,XZO,YNOO,TO,RATES,TB,G2,Y2,XZ2,YNO2,T2,
                 1                   NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB,SS,TI)
            C
            C
            C
            C
            C*******************************************************
            C*    THIS SUBROUTINE MIXES THE GAS STREAM AND THE     *
            C*    FUEL STREAM TO COMPUTE A NEW TEMPERATURE AND     *
            C*    COMPOSITION.--IN THE TEMPERATURE CALCULATION     *
            C*    THE HEAT OF VAPORIZATION/GASIFICATION IS TAKEN   *
            C*    INTO ACCOUNT.                                    *
            C*******************************************************
            C
            C
            C
 0002             DIMENSION ICODE( 6),YO( 2),XZO( 4),Y2(2),XZ2(4),CPCOEF(NCOMP,10),
                 1          CPAVG(NCOMP),XMOLE(6),YFUEL(2),XFUEL(4)
 0003             COMMON/AA/HVAP
 0004             COMMON/BB/TIME
            C     YO=MOLE FRACTION OF INDEPENDENT COMPONENT AT THE BEGGINING
            C        OF THE SLICE
            C     XZO=SIMILAR TO YO BUT FOR THE INDEPENDENT COMPUNENTS
            C     Y2=MOLE FRACTION OF IND. COMP. AT EXIT OF SLICE
            C     XZ2=MOLE FRACTICN OF DEP. COMP. AT EXIT OF SLICE
            C
            C
 0005         999 CONTINUE
 0006             NTOTAL=NIND + NDEP
            C
            C
 0007             YNOFL=0.
 0008             YFUEL(1)=0.
 0009             YFUEL(2)=0.
 0010             XFUEL(1)=1.0
 0011             XFUEL(2)=0.
 0012             XFUEL(3)=0.
 0013             XFUEL(4)=0.
            C
 0014             TR=298.
 0015             CALL MIX(GO,YO,XZO,YNOO,TO,RATES,YFUEL,XFUEL,YNOFL,TI,G2,Y2,XZ2,
                 1        YNO2,T2,NIND,NDEP,NCOMP,CPAVG,CPCOEF,IBCMB)
 0016             HEAT=RATES*HVAP
 0017             IF(SS .NE. 0.) GO TO 710
 0018             CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,TB)
 0019             XCP4=CPAVG(4)
 0020             SNSBL=RATES*CPAVG(4)*(TB-TI)
 0021             TI=TB
 0022             HEAT=HEAT+SNSBL
 0023         710 CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,T2)
 0024             CPMIX2=0.
 0025             DO 30 I=1,NTOTAL
 0026             IF(I.GT. NIND) GO TO 29
```

```
FORTRAN IV G LEVEL  20                 UPDATE                                          PAGE 0002
      CPMIX2=CPMIX2+Y2(I)*CPAVG(I)
      GO TO 30
   29 II=I-NIND
      CPMIX2=CPMIX2+XZ2(II)*CPAVG(I)
   30 CONTINUE
      DELT=HEAT/(G2*CPMIX2)
      T2=T2-DELT
      PRINT 90,T2,DELT
   90 FORMAT(//1X,'T2=',E14.6,'DELT=',E14.6/)
      RETURN
      END
```

```
FORTRAN IV G LEVEL  20                  SPRAY                                                        PAGE 0001

0001                 SUBROUTINE SPRAY(AREA,STEP,RATES,NT,NSPRAY,TB,T,P,G)
              C
0002                 DIMENSICN AREAPO(10),EVAP(10),BURN(10),ERATE(10)
0003                 DIMENSION RF(10),RF2(10),RF3(10)
0004                 DIMENSICN W(10)
0005                 DOUBLE PRECISION EERATE
              C
              C**** THIS SUBROUTINE COMPUTES THE MOLES/SEC OF
              C     GAS GENERATED BY EITHER THE BURNING OF A
              C     LIQUID SPRAY OR A SCLID SPRAY
              C
0C06                 COMMON/AB/R(10),RHONV(10),NGROUP,NFNCTN,RHOP,AVGMW,
                    1          VP,     WDP(10),XNDP(10)
0007                 COMMON /EE/ FUEL
              C
              C      THE COMMON BLOCK /AB/ IS LINKED TO SUBROUTINE ADATA
              C
0L08                 REAL K
              C
              C        AVGMW=AVERAGE MOLECULAR WEIGHT OF GAS GIVEN OFF
              C        AREA=CROSS SECTIONAL AREA OF FLOW(FT**2)
              C        ERATE=EVAPORATION RATE OF LIQUID SPRAY,OR
              C              GASIFICATION RATE OF SOLIDS(MOLES/SEC). ERATE IS
              C        NSPRAY=1 (SPRAY IS LIQUID)
              C        NSPRAY=2 (SPRAY IS SOLID)
              C        NT=COUNTER
              C        R(I)=PARTICLE RADIUS (MICRONS)
              C        RHOP=PARTICLE DENSITY. ASSUMED TO BE
              C             UNIFORMED FOR ALL PARTICLES(LBS/FT**3)
              C        VP=PARTICLE VELOCITY(FT/SEC)
              C        NGROUP=NO. OF DISCRETE PARTICLE SIZES GROUPS
              C               USED TO CHARACTERIZE THE DISTRIBUTION
              C               OF THE SPRAY. IT CANNOT EXCEED 10.
              C
0009                 PI=3.1416
0010                 XSQR4P=SQRT(4.*PI)
              C
              C        NFNCTN=0  VAPORIZATION/GASIFICATION RATE IS CONSTANT
              C        NFNCTN=1  VAPORIZATION/GASIFICATION RATE IS NOT CONSTANT
              C        FUEL=TOTAL MOLES OF LIQUID/SOLID FUEL FED TO BOILER
              C        P=PRESSURE(PSI)
              C
              C**** INITIALIZATION
              C
              C
0011                 IF(NT.NE.0)GO TO 3
              C      FPI=4.*PI
0012                 FPI=12.5664
0013                 RR=1206.28
              C      RR=1206.28(CM**3-PSI/(GM-MOLE OK)
0014                 TFUEL=FUEL
0015                 SUMFUL=0.
              C
```

```
             C       WDP=WEIGHT DISTRIBUTION OF PARTICLES
             C       XNDP=NUMBER DISTRIBUTION OF PARTICLES/SEC
             C
 0016              PI43RO=PI*4./3.*RHOP
 0017              FAVGMW=FUEL*AVGMW
             C
             C******** CALCULATE THE PARTICLES/SEC OF FUEL XNDP(I) FOR
             C           EACH GROUP OF PARTICLES BEING FED INTO THE BURNER.
             C           FORM THE CONTINUITY EQUATION WE KNOW THAT XDNP(I)
             C           IS CONSTANT.
             C
 0018              DO 1 I=1,NGROUP
             C
             C------- CONVERT FROM MICRONS TO FEET
             C
 0019              RF(I)=R(I)/30.48E4
 0020              RF2(I)=RF(I)*RF(I)
 0021              RF3(I)=RF(I)*RF2(I)
 0022              AREAPO(I)=FPI*RF2(I)
 0023            1 XNDP(I)=WDP(I)*FAVGMW/PI43RO/RF3(I)/454.
             C
             C     1 MICRON= 1./30.48E4 FEET
             C
             C     IF THE SPRAY IS A SOLID BYPASS LIQUID SPRAY CALCULATION.
             C
             C
             C
             C******** CALCULATE THE VELOCITY OF THE FUEL PARTICLES. IT
             C           IS ASSUMED THAT THESE PARTICLE MOVE AT THE VELO-
             C           CITY OF THE GAS STREAM ENTERING THE DIFFERENTIAL
             C           ELEMENT.
             C
 0024            3 VP=G*RR*T/P/28320./AREA
             C
             C
             C-------- SUBROUTINE VAPOR CALCULATES THE EVAPORATION
             C           RATE,EVAP, PER UNIT AREA OF LIQUID FOR EACH
             C          GROUP OF PARTICLES.
             C
 0025              CALL VAPOR(RF,PI,VP,RHOP,STEP,NGROUP,W)
             C
 0026              WW=0.
 0027              DO 27 I=1,NGROUP
 0028              WW=WW + W(I)*XNDP(I)
 0029           27 CONTINUE
 0030              WW=WW*454./AVGMW
 0031              RATES=WW
 0032              EERATE=-WW
 0033              SUMFUL=SUMFUL-EERATE
 0034              IF(SUMFUL.GE.TFUEL)NSPRAY=0
 0035              IF(SUMFUL.GT.TFUEL)RATES=RATES-(SUMFUL-TFUEL)
 0036              DIVI=SUMFUL/TFUEL
 0037              IF(DIVI.GE.0.9999)NSPRAY=0
```

```
      NT=NT+1
      IF(RATES.LT.1.)NSPRAY=0
      PRINT 30
   30 FORMAT(/2X,'PARTICLE RADIUS PARTICLE SURFACE EVAPORATION RATE DENS
     1ITY FUNCTION PARTICLE VELOCITY  NO. OF GROUPS'/)
      DO 50 I=1,NGROUP
      R(I)=RF(I)*30.48E4
      PRINT 31,R(I),VP,WW,NGROUP
   31 FORMAT(1X,3E17.7,7X,I3)
   50 CONTINUE
      RETURN
      END
```

```
FORTRAN IV G LEVEL  20                VAPOR                                                 PAGE 0001
 0001              SUBROUTINE VAPOR(RF,PI,VP,RHOP,STEP,NGROUP,W)
             C
             C  THIS SUBROUTINE CALCULATES THE VAPORIZATION OF FUEL OIL DROPLETS
             C
 0002              COMMCN /IJ/ VAPF
 0003              DIMENSION DELTA(10), D(10), DNEW(10), RF(10), W(10)
 0004              COMMON/BB/TIME
 0005              PRINT 50
 0006           50 FORMAT (2X, 'NGROUP', 5X, 'D', 10X, 'DNEW', 10X, 'DELTA', 10X,
                 1  'W', 12X, 'EVAP')
 0007          400 CONTINUE
 0008              X1=VAPF
 0009              DELT=STEP/VP
 0010              TIME=TIME + DELT
 0011              GROUP5=VAPF*TIME
 0012              DO 200 I = 1,NGROUP
 0013              D(I)=RF(I)*2.
             C
             C  CALCULATE NEW DIAMETER
             C
 0014              ARG =  D(I)**2 -  GROUP5
 0015              IF (ARG .LE. 0.0) ARG=1.E-40
 0016              DNEW(I) = SQRT(ARG)
             C
             C  CALCULATE CHANGES IN SURFACE
             C
 0017              DELTA(I)=PI*D(I)**2
             C
             C  CALCULATE TOTAL LBS EVAPORATED
             C
 0018              W(I) = RHOP * (PI/6) * (D(I)**3 - DNEW(I)**3)
             C
             C  CALCULATE VAPORIZATION FLUX
             C
             C     EVAP(I)=W(I)/DELTA(I)/DELT
             C
             C  PRINT RESULTS
             C
 0019              RF(I)=DNEW(I)/2.
 0020              PRINT 100,I,D(I),DNEW(I),DELTA(I),W(I)
 0021          100 FORMAT ( 4X, I2, 5(1X, E12.5))
 0022          200 CONTINUE
 0023              RETURN
 0024              END
```

```
FORTRAN IV G LEVEL  20                  POLUT                                                   PAGE 0001

0001              SUBROUTINE POLUT(P,T,GOLD,G,YNOLD,STEP,A,YN2,YO2,YNO,YNOEQ,SS,
                 1         MACRO)
0002              DOUBLE PRECISION ONE,TWO,FOUR,AAA,CCC,DELTAA,YYNO1,YYNO2,XXSQR
0003              DOUBLE PRECISION VLUME,GG, AA4,AA2,YYO2,GGOLD,YYNOLD,AA3,AA1,
                 1                 YYN2,XDSO2,APRME,BPRME,CPRME,SSS
0004              DOUBLE PRECISION GROUP1,GROUP3,DNODT,YYNO,YYO2EQ
0005              COMMON /PCLMCR/ DNODTT,VOLUME
0006              CCMMON/CD/YO2EQ
0007              COMMON/EF/TEST1,KINJEC,KPASSS
            C
            C**** THIS SUBROUTINE COMPUTES THE MOLE FRACTION OF NITROGEN OXIDE ****
            C
            C     A=AREA OF FLOW(FT**2)
            C
            C     A=AREA OF FLOW(FT**2)
            C     G=MCLAR FLOW RATE OF GASES (MOLES/SEC)
            C     GOLD= MOLAR FLOW RATE OF GASES IN PREVIOUS SLICE
            C     YNO=MOLE FRACTION OF NO
            C     YNOEQ=EQUILIBRIUM MOLE FRACTION
            C     YNOLD=MOLE FRACTION OF NO IN PREVIOUS STEP
            C     YO2=MOLE FRACTION OF OXYGEN
            C     YN2=MOLE FRACTION OF NITROGEN
            C     P=PRESSURE(PSIA)
            C     T=TEMPERATURE(OK)
            C     STEP=INTEGRATION STEP SIZE(IN FEET)
            C     SS=DISTANCE FROM THE INLET(FEET)
            C     VLOCT=VELOCITY CF GAS(FT/SEC)
            C     YO2EQ=EQUILIBRIUM MOLE FRACTION OF OXYGEN
            C     XKO=EQUILIBRIUM OXYGEN DISSOCIATION CONSTANT
            C
0008              IF (MACRO .GT. 0) GO TO 1
0009              IF(KPASSS.EQ.1)GO TO 1
0010              IF(KINJEC.EQ.0.AND.YO2.LT.YO2EQ)YO2=YO2EQ
0011            1 RR=1206.28
            C
            C     RR=1206.28(CM**3-PSI/(OK-GM-MOLE))
0012              R=1.987
            C     R=1.987(CALORIES/(GM-MOLE-OK))
0013              PRT=P/(RR*T)
0014              PRT25=PRT**2.50C
            C
            C**** COMPUTE THE MOLE FRACTION OF NO
            C
            C     GOLD*YNOLD - G*YNO +A*STEP*RATE OF NO = 0
            C     THE ABOVE EXPRESSION IS THE DIFFERENTIAL
            C     MASS BALANCE ON NO
            C
0015              XKO=25.*EXP(-118600./(R*T))
0016              RT=R*T
            C
            C-------- LEEDS DATA
            C
0017              XK3=1.36E14*EXP(-75400./(R*T))                                    LEEDS
```

```
FORTRAN IV G LEVEL  20                POLUT                                                      PAGE 0002
 0018             XK4=3.1E13*EXP(-334./(R*T))                                        LEEDS
 0019             XK5=6.43E9*T*EXP(-6250./(R*T))                                     LEEDS
 0020             XK6=1.55E9*T*EXP(-38640./(R*T))                                    LEEDS
 0021             A1=2.*SQRT(XKO)*XK3*XK5*PRT25
 0022             A2=2.*SQRT(XKO)*XK4*XK6*PRT25
 0023             A3=XK5*PRT
 0024             A4=XK4*PRT
 0025             AA1=A1
 0026             AA2=A2
 0027             AA3=A3
 0028             AA4=A4
            C
            C
 0029             VOLUME=A*STEP*28320.
 0030             VLUME=VOLUME
            C
            C         THE FACTOR 28320. IS TO CONVERT FROM CM**3 TO FT**3.
            C
 0031             GG=G
 0032             YYO2=YO2
 0033             GGOLD=GOLD
 0034             YYNOLD=YNOLD
 0035             YYN2=YN2
 0036             XDSO2=DSQRT(YYO2)
 0037             GROUP1=AA1*YYN2*YYO2*XDSO2
 0038             GROUP3=AA3*YYO2
 0039             APRME=-(GG*AA4 + VLUME*AA2*XDSO2)
 0040             BPRME=GGOLD*YYNOLD*AA4-GG*GROUP3
 0041             CPRME=GGOLD*YYNOLD*GROUP3 + VLUME*GROUP1
 0042             AAA=APRME/BPRME
 0043             CCC=CPRME/BPRME
 0044             VLOCT=G/PRT/28320./A
 0045             ONE=1.0000000
 0046             TWO=2.0000000
 0047             FOUR=4.0000000
 0048             DELTAA=FOUR*AAA*CCC
 0049             XXSQR=DSQRT(ONE-DELTAA)
 0050             YYNO1=(-CNE+XXSQR)/(TWO*AAA)
 0051             YYNO2=(-ONE-XXSQR)/(TWO*AAA)
            C
            C
            C---------FIND VALID ROOT
            C
 0052             IF(YYNO1.GE.0..AND.YYNO1.LT.1.)YYNO=YYNO1
 0053             IF(YYNO2.GE.0..AND.YYNO2.LT.1.)YYNO=YYNO2
 0054             YNO=YYNO
            C
            C---------CORRECT OXYGEN CONCENTRATION BY SUBTRACTING AMOUNT
            C         CONSUMED BY THE NITROGEN OXYGEN REACTION.
            C
            C
            C         DNOOT=GENERATION RATE OF NITROGEN OXIDE(GM-MOLES/CM**3-SEC)
            C
```

```
C
    2 YNOEQ= 4.68*EXP(-21700./(R*T))*(YN2**0.5)*(YO2**0.5)
      IF(SS.EQ.0.)TIME=0.
      DLTIME=STEP/VLOCT
      TIME=TIME+DLTIME
      DNODT=(GROUP1-AA2*YYNC**2*XDSO2)/(GROUP3+AA4*YYNO)
      DNUDTT=DNODT
      IF(MACRO.GT.0)RETURN
      IF(SS.LT.TEST1)RETURN
      IF(KPASSS.EQ.0)GO TO 3
      IF(KINJEC.EQ.1)YO2EQ=YO2
      IF(KINJEC.EQ.1)YYO2EQ=YO2EQ
      IF(KINJEC.EQ.1)KINJEC=0
      YYO2EQ=YYO2EQ-DNODT*VLUME/GG/2.
      YO2EQ=YYO2EQ
      YC2=YO2EQ
      RETURN
    3 CONTINUE
      IF(YO2EQ.EQ.0.)YO2EQ=YO2
      YYO2=YO2EQ
      YYO2=YYO2-DNODT*VLUME/GG/2.
      IF(YYO2.LT.0.)YYO2=0.
      YO2EQ=YYO2
      YO2=YYO2
      RETURN
      END
```

D.2 Particle Combustion

D.2.1 Input Forms for Particle Combustion

PARTICLE COMBUSTION

CARD 0 TITLE CARD

COLUMNS
1 - 80

CARD 1 OPTION CODES

COLUMN	
1-5	IS WALL TEMPERATURE PROFILE TO BE SPECIFIED ? (*)
6-10	IS GAS TEMPERATURE PROFILE TO BE SPECIFIED ? (**)
11-15	IS HEAT FLUX PROFILE TO BE SPECIFIED ? (*)
16-20	NUMBER OF SECONDARY INJECTION POINTS (MAXIMUM OF 20)
21-25	NSPRAY PARAMETER ***
26-30	
31-35	
36-40	
41-45	
46-50	
51-55	
56-60	
61-65	
66-70	

(*) { 1 = YES, BY USER
0 = NO

ALL ITEMS ON THIS CARD MUST BE RIGHT-JUSTIFIED.

(**) { 0 = NO
1 = YES, BY USER
2 = YES, FROM QUENCH RATE CALCULATIONS

ONE, AND ONLY ONE, OF THE 3 SPECIFICATION OPTIONS MAY BE EXERCISED - i.e., ONLY ONE "YES" RESPONSE.

*** { 0 = FUEL IS A GAS
1 = FUEL IS A LIQUID
2 = FUEL IS A SOLID

CARD 2 STOICHIOMETRIC COEFFICIENTS FOR $a(\text{FUEL}) + b(O_2) \rightarrow c(CO) + d(H_2O)$

COLUMN		
1-10	.	FUEL COEFFICIENT, a
11-20	.	O_2 " , b
21-30	.	CO " , c
31-40	.	H_2O " , d
41-50		
51-60		
61-70		

CARD 3 PHYSICAL CONDITIONS OF INLET GAS MIXTURE

COLUMN		
1-10	.	FLOW RATE (g-MOLES / SECOND)
11-20	.	TEMPERATURE (°K)
21-30	.	PRESSURE (PSIA)
31-40	.	ADIABATIC FLAME TEMPERATURE AT INLET (
41-50		
51-60		
61-70		

CARD 4 INLET GAS COMPOSITION

COLUMN		
1-10	.	MOLE FRACTION OF O_2
11-20	.	" CO_2
21-30	.	" FUEL
31-40	.	" CO
41-50	.	" H_2O
51-60	.	" N_2
61-70	.	" NO

NOTES:

(*) OPTIONAL - USED IN CONJUNCTION WITH QUENCH RATE

CARD 5 CONDITION AND LOCATION OF SECONDARY INJECTION GAS

COLUMN		
1-10	.	FLOW RATE (g-MOLES / SEC.)
11-20	.	TEMPERATURE (°K)
21-30	.	INJECTION POINT (FEET FROM INLET)
31-40	.	ADIABATIC FLAME TEMP. AT INJECTION (°K)
41-50		(If left blank will [illegible])
51-60		
61-70		

CARD 6 INJECTION GAS COMPOSITION

COLUMN		
1-10	.	MOLE FRACTION OF O_2
11-20	.	" CO_2
21-30	.	" FUEL
31-40	.	" CO
41-50	.	" H_2O
51-60	.	" N_2
61-70	.	" NO

(*) OPTIONAL - USED IN CONJUCTION WITH QUENCH RATE.

NOTES:

A MAXIMUM OF 20 INJECTION POINTS MAY BE USED.

IF NO INJECTION POINTS ARE USED, DO NOT SUBMIT THESE CARDS

INJECTION POINTS MUST BE SUBMITTED IN ORDER OF INCREASING DISTANCE FROM [illegible]

USE ADDITIONAL CARDS AS NEEDED FOR MORE INJECTION POINTS.

CARD 7 KINETIC RATE CONSTANTS FOR a (FUEL) + b (O_2) → c (CO) + d (H

COLUMN		
1-10		FREQUENCY FACTOR, A (*)
11-20		ACTIVATION ENERGY, E (CALORIES)
21-30		O_2 EXPONENT, α
31-40		FUEL " , β
41-50		H_2O " , γ
51-60		
61-70		

THE KINETIC RATE EXPRESSION IS -

$$\mathcal{R} = A\, e^{-\frac{E}{RT}} (O_2)^{\alpha} (\text{FUEL})^{\beta} (H_2O)^{\gamma} \quad \text{g-MOLES/LITER-SEC;}$$

WITH (O_2), (FUEL) AND (H_2O) IN UNITS OF g-MOLES/LITER AND T IN °K.

(*) THIS ITEM MAY BE EXPRESSED AS AN EXPONENTIAL NUMBER, 0.XXXXE±

CARD 8 KINETIC RATE CONSTANTS FOR $CO + \frac{1}{2} O_2 \rightarrow CO_2$

COLUMN		
1-10		FREQUENCY FACTOR, A (*)
11-20		ACTIVATION ENERGY, E (CALORIES)
21-30		O_2 EXPONENT, α
31-40		CO " , β
41-50		H_2O " , γ
51-60		
61-70		

THE KINETIC RATE EXPRESSION IS -

$$\mathcal{R} = A\, e^{-\frac{E}{RT}} (O_2)^{\alpha} (CO)^{\beta} (H_2O)^{\gamma} \quad \text{g-MOLES/LITER-SEC;}$$

WITH (O_2), (CO) AND (H_2O) IN UNITS OF g-MOLES/LITER AND T IN °K.

CARD 9 HEAT TRANSFER CONSTANTS

COLUMN		
1-10	.	CONSTANT COEFFICIENT, A
11-20	.	CONVECTION ", B
21-30	.	RADIATION ", C
31-40		
41-50		
51-60		
61-70		

THE HEAT FLUX TO THE WALL IS EXPRESSED AS –

$$q \text{ (KCAL./FT}^2\text{-SEC)} = A + B(T - T_w) + C(T^4 - T_w^4),$$

WHERE T AND T_w ARE THE GAS AND WALL TEMPERATURES (°K

THIS CARD IS TO BE SUBMITTED ONLY IF THE WALL TEMPERATURE SPECIFICATION OPTION HAS BEEN EXERCISED ON CARD 1 (A "1" IN COLUMN 5).

CARD 9.5 QUENCH RATE CONSTANTS

COLUMN		
1-10	.	FIRST COEFFICIENT, A
11-20	.	SECOND " , B
21-30	.	THIRD " , C
31-40	.	FORM OF QUENCH RATE (*)
41-50		
51-60		
61-70		

(*) { 0.0 = QUADRATIC FORM
1.0 = EXPONENTIAL FORM

QUADRATIC FORM : $A + BT + CT^2$

EXPONENTIAL FORM : $(A + BT)\, e^{C/T}$

(T IN °K
QUENCH RATE IN °K/SEC)

THIS CARD IS TO BE SUBMITTED ONLY IF THE GAS TEMPERATURE IS TO BE COMPUTED FROM A QUENCH RATE (A "2" IN COLUMN 10 ON CARD 1).

omit for [illegible]

CARD 10 COMBUSTOR PROFILES

COLUMN		
1-10	DISTANCE FROM INLET (FEET)	
11-20	CROSS-SECTIONAL AREA (FT^2)	
21-30	PERIMETER (FEET)	
31-40	WALL TEMPERATURE (°K)	(**)
41-50	GAS TEMPERATURE (°K)	
51-60	HEAT FLUX ($KCAL/FT^2$-SEC)	
80	(*)	

CARD 10 COMBUSTOR PROFILES

COLUMN		
1-10	DISTANCE FROM INLET (FEET)	
11-20	CROSS-SECTIONAL AREA ($FT.^2$)	
21-30	PERIMETER (FEET)	
31-40	WALL TEMPERATURE (°K)	(**)
41-50	GAS TEMPERATURE (°K)	
51-60	HEAT FLUX ($KCAL/FT^2$-SEC)	
80	(*)	

(*) ENTER A "1" IN COLUMN 80 IF THIS IS THE FINAL PROFILE CARD.

(**) ENTER VALUES FOR THE ITEM CORRESPONDING TO THE SPECIFICATION CHOSEN ON CARD 1.

AT LEAST TWO CARDS, ONE FOR THE INLET AND ONE FOR THE OUTLET, MUST ALWAYS BE SUBMITTED (MAXIMUM OF 100 CARDS).

USE ADDITIONAL CARDS AS NEEDED FOR MORE PROFILES.

PROFILE CARDS MUST BE SUBMITTED IN ORDER OF INCREASING DISTANCE FROM INLET.

CARD 11 COMBUSTOR LENGTH AND PRINTOUT INTERVAL

COLUMN	
1-10	REACTOR LENGTH (FEET)
11-20	PRINTOUT INTERVAL (FEET) (*)
21-30	INTEGRATION INTERVAL (FEET) (**)
31-40	
41-50	
51-60	
61-70	

(*) A NUMBER, N, ENTERED HERE WILL CAUSE RESULTS TO BE PRINTED OUT EVERY N FEET ALONG THE COMBUSTOR. THIS NUMBER SHOULD BE AT LEAST AS LARGE AS THE INTEGRATION INTERVAL.

(**) IF LEFT BLANK, THE INTEGRATION INTERVAL WILL BE ASSUMED TO BE 1/120 TH OF THE LENGTH OF A FLAME SEGMENT.

CARD 12 HEAT OF REACTION @ 298 °K

COLUMN	
1-10	HEAT OF REACTION (KCAL) FOR REACTION ON CARD 7
11-20	HEAT OF REACTION (KCAL) FOR REACTION ON CARD 8
21-30	
31-40	
41-50	
51-60	
61-70	

CONVENTION: EXOTHERMIC HEAT OF REACTION MUST BE ENTERED AS A NEGATIVE NUMBER.

CARD 13 HEAT CAPACITY DATA FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN					
1-4					NUMBER OF HEAT CAPACITY DATA POINTS FOR FUEL (*) (298°K ≤ T ≤ 1200°K
5-8					
9-12					
13-16					
17-20					
21-24					
25-28					
29-32					
33-36					
37-40					
41-44					
45-48					
49-52					
53-56					
57-60					
61-64					
65-68					
69-72					

NOTES:

AT LEAST 6 DATA POINTS, INCLUDING VALUES AT 298°K AND 1200°K, MUST BE SUBMITTED. IT IS RECOMMENDED THAT AT LEAST 10 POINTS BE USED (MAXIMUM OF 20).

(*) THIS NUMBER MUST BE RIGHT-JUSTIFIED.

CARD 14 HEAT CAPACITY DATA POINTS FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN		
5-14	.	TEMPERATURE (°K)
15-24	.	HEAT CAPACITY OF FUEL (CAL/g-MOLE-°K)

CARD 14 HEAT CAPACITY DATA POINTS FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN		
5-14	.	TEMPERATURE (°K)
15-24	.	HEAT CAPACITY OF FUEL (CAL/g-MOLE-°K)

CARD 14 HEAT CAPACITY DATA POINTS FOR FUEL (298°K ≤ T ≤ 1200°K)

COLUMN		
5-14	.	TEMPERATURE (°K)
15-24	.	HEAT CAPACITY OF FUEL (CAL/g-MOLE-°K)

NOTES:

AT LEAST SIX DATA CARDS MUST BE SUBMITTED, INCLUDING VALUES AT 298°K AND 1200°K. DATA CARDS MUST BE SUBMITTED IN ORDER OF INCREASING TEMPERATURES.

USE ADDITIONAL CARDS AS NEEDED FOR MORE DATA POINTS.

CARD 15 HEAT CAPACITY DATA FOR FUEL (T > 1200°K)

COLUMN					
1-4					NUMBER OF HEAT CAPACITY DATA POINTS FOR FUEL (*)
5-8					(T > 1200°K)
9-12					
13-16					
17-20					
21-24					
25-28					
29-32					
33-36					
37-40					
41-44					
45-48					
49-52					
53-56					
57-60					
61-64					
65-68					
69-72					

NOTES:

AT LEAST 6 DATA POINTS MUST BE SUBMITTED. IT IS RECOMMENDED THAT AT LEAST 10 POINTS BE USED (MAXIMUM OF VALUES ABOVE 3000°K ARE USUALLY NOT NEEDED.

(*) THIS NUMBER MUST BE RIGHT-JUSTIFIED.

CARD 16 HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200 °K)

COLUMN	
5-14	TEMPERATURE (°K)
15-24	HEAT CAPACITY OF FUEL (CAL/g-MOLE - °K)

CARD 16 HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200 °K)

COLUMN	
5-14	TEMPERATURE (°K)
15-24	HEAT CAPACITY OF FUEL (CAL/g-MOLE · °K)

CARD 16 HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200 °K)

COLUMN	
5-14	TEMPERATURE (°K)
15-24	HEAT CAPACITY OF FUEL (CAL/g-MOLE · °K)

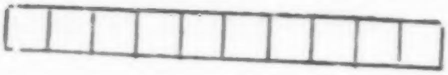
NOTES:

AT LEAST SIX DATA CARDS MUST BE SUBMITTED FOR VALUES ABOVE 1200 °K. DATA CARDS MUST BE SUBMITTED IN ORDER OF INCREASING TEMPERATURES.

USE ADDITIONAL CARDS AS NEEDED FOR MORE DATA POINTS.

CARD 17 Oxygen Equilibrium Restriction

COLUMN
1 - 10



EVEN WHEN NO RESTRICTIONS ARE IMPOSED BLANK CARD MUST BE INCLUDED. E FIELD IS USED. MUST BE RIGHT HAND JUSTIFIED

CARD 18 NON-GASEOUS FUEL PARAMETER CARD

Column	
1-2	ICØDE(1)*
3-4	ICØDE(2)
5-6	ICØDE(3)
6-7	ICØDE(4)
8-9	ICØDE(5)
9-10	ICØDE(6)
11-13	NFNCTN **
13-15	No. of Groups of PARTICLE in Spray Distrib
16-25	DENSITY OF FUEL
26-35	MOLECULAR WEIGHT OF Fuel
36-45	Boiling Point of Fuel Oil
46-55	HEAT OF VAPORIZATION

* WHEN ICØDE = 1 THE SPECIE IS NON-GASEOUS

** WHEN NFNCTN = 0 VAPORIZATION RATE IS CONSTANT
= 1 VAPORIZATION RATE IS A FUNCTIO DEFINED BY THE USER

CARD 19: PARTICLE Distribution

Columns	
1-10	RADIUS OF PARTICLES IN SPRAY (MICRONS)
11-20	WEIGHT DISTRIBUTION FUNCTION

REPEAT DEPENDING ON THE NUMBER OF POINTS USED TO DESCRIBE A PARTICLE DISTRIBUTION FUNCTION.

D.2.2 Computer Listing for Particle Combustion

```
FORTRAN IV G LEVEL  19                  MAIN                                                     PAGE 0001
 0001              DIMENSION DABINV(2),YO(2),Y(2),YOLD(2),GAMBIV(4,2),B(2,2),XZO(4)
 0002              DIMENSION GAMMA(4,2),BINV(2,2) ,YO(2),XZOLD(4)
 0003              DIMENSION DELALP(2),CPCOEF(6,10),           DGIDY(2),DXZDY(4,2)
 0004              DIMENSION DCOF(2,14)
 0005              DIMENSION R(2),DRDY(2,2),DRDXZ(2,4),DRDT(2),CP(6),DCPDT(6)
 0006              DIMENSION DGCPDY(2),DELH(2),DHDT(2),LMINV(3),MMINV(3),XZ(4)
 0007              DIMENSION AJACOB(3,3),FUN(3)
 0008              DIMENSION XPOINT(100),AREA(100),PERIM(100),TWALL(100)
 0009              DIMENSION TSPEC(100),QSPEC(100),KODE(4)
 0010              DIMENSION HTC(3),    RCON(10)
 0011              DIMENSION TX(20),CPY(20),C(4),FO(4),F(20,4),A(4,4)
 0012              DIMENSION XINJ(20),GINJ(20),TINJ(20),YINJ(2,20),XZINJ(4,20)
 0013              DIMENSION YNOINJ(20)
 0014              DIMENSION Y2(2),XZ2(4),CPAVG(6)
 0015              DIMENSION QNCHRT(3), TCOMBI(20)
 0016              DIMENSION ICODE(6)
 0017              COMMON/BB/TIME
 0018              COMMON/EF/TEST1,KINJEC,KPASSS
 0019              DATA CPCOEF/   7.316 ,    4.102,      0.0,     7.705,      8.613,
                 1     7.681,  -4.363 ,   22.07 ,      0.0,    -5.617,     -2.632,
                 2    -5.146,  15.23  ,  -24.55 ,      0.0,    13.32 ,      9.036,
                 3    11.42 , -14.26  ,   15.47 ,      0.0,   -10.22 ,     -6.405,
                 4    -8.253,   4.429 ,   -4.1  ,      0.0,     2.744,      1.688,
                 5     2.108,  16.67  ,   15.96 ,      0.0,     9.867,     22.94 ,
                 6    10.01 , -24.12  ,   -4.295,      0.0,    -5.465,    -63.02 ,
                 7    -6.693,  49.93  ,    4.718,      0.0,    11.86 ,    154.3  ,
                 8    15.06 , -50.14  ,   -5.741,      0.0,   -14.76 ,   -181.7  ,
                 9   -18.80 ,  19.29  ,    2.321,      0.0,     6.559,     78.85 ,
                 A     8.405/
            C
            C
            C*******************************************
            C*    MODIFIED FOR BURNING OF SPRAY PARTICLES    *
            C*******************************************
            C
            C
 0020              CALL RELOC
 0021           40 CONTINUE
 0022              IBOMB=0
 0023              NOPT = 4
 0024              NIND = 2
 0025              NDEP = 4
 0026              NDIM = 3
 0027              NCOMP = 6
 0028              SS=0.
 0029              TIME=0.
 0030              KPASSS=0
 0031              KINJEC=0
 0032              NT=0
 0033              CALL         ADATA(NIND,NDEP,NCOMP,B,GAMMA,YO,XZO,CPCOEF,DCOF,YNOO,
                 1                   CP,DCPDT,DELH,DHDT,RCON,HTC,XPOINT,AREA,PERIM,
                 2                   TWALL,TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
                 3                   PINT,XINJ,GINJ,TINJ,YINJ,XZINJ,YNOINJ,
                4                     NOPT,TX,CPY,C,FO,F,A,QNCHRT,QNCHTP,TCOMB,TCOMBI,
                5                     NSPRAY,ICODE,TB)
 0034            TEST1=3.*DELTAX
 0035            C1=-GAMMA(1,1)
 0036            C2=-B(1,1)
 0037            C1= -GAMMA(2,2)
 0038            C2= -B(1,2)
          C         FORM THE ARRAY DELALP WHOSE J'TH ELEMENT CONTAINS THE NET
          C         CHANGE IN MCLES FOR THE J'TH REACTION.
 0039            DO 1 JJ= 1,NIND
 0040            DELALP(JJ)= 0.
 0041            DO 2 II = 1,NIND
 0042          2 DELALP(JJ) = DELALP(JJ)+ B(II,JJ)
 0043            DO 1 II = 1,NDEP
 0044          1 DELALP(JJ) = DELALP(JJ)+GAMMA(II,JJ)
          C         CALCULATE THE INVERSE OF THE 'INDEPENDENT' STOICHIOMETRIC
          C         MATRIX.
 0045            CALL BINVER(NIND,B,BINV)
          C      PREMULTIPLY THE INVERSE OF B BY GAMMA, THE 'DEPENDENT'
          C      STOICHIGMETRIC MATRIX.
 0046            CALL MPRD(GAMMA,BINV,GAMBIV,NDEP,NIND,0,0,NIND)
          C      PRIMULTIPLY THE INVERSE  OF B BY DELALP
 0047            DO 3 JJ = 1,NIND
 0048            DABINV(JJ) = C.
 0049            DO 3 II = 1,NIND
 0050          3 DABINV(JJ)=DABINV(JJ) + DELALP(II)*BINV(II,JJ)
          C
          C         FOR LIQUID CR SOLID FUELS XZO(1) IS READ IN AS ZERO.
          C         THEREFCRE, THE COMPUTATION OF THE ADIABATIC FLAME
          C         TEMPERATURE MOST BE PCSTPCNED UNTIL SOME FUEL IS AL-
          C         LOWED TO VAPORIZE.
          C
          C
 0051            IF(NSPRAY.NE.C)GC TO 502
 0052            CALL THERMC(TC,NIND,NCCMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
 0053            CALL TADB(NIND,NDEF,NCCMP,YO,XZO,Y,XZ,DELH,DELALP,B,GAMMA,
               1          CPCCEF,CPAVG,GO,G,TO,TACAB,HEAT)
 0054            PRINT 50C, TADAB
 0055        500 FORMAT (1H1, 58X, 'CCMBUSTION/POLLUTION MODEL',// 64X, 'OUTPUT',
               1        ' SUMMARY',// 57X, 28('*'),////T20, 'ADIABATIC FLAME ',
               2        'TEMPERATURE FOR INLET GAS MIXTURE = ', F10.2, ' K',/)
 0056        502 IF(KODE(4).LE.0)GC TO 50
 0057            XFIN = XINJ(1)
 0058            CALL        INTGRT(NIND,NDEP,NDIM,NCCMP,DABINV,YO,YOLD,Y,GAMBIV,B,
               1                    GAMMA,YC,XZOLD,YNOO,YNO,G,T,TB,
               2                    XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
               3                    DRDT,RCCN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
               4                    MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
               5                    TSPEC,QSPEC,KODE,GO,P,TO,XO,XFIN,DELTAX,
               6                    PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
               7                   NSPRAY,ICODE,SS,NT)
 0059            IF(IBOMB.NE.0) GO TO 40
 0060            KINJ = 0
```

```
      35 KINJ = KINJ+1
         IF(KINJ .GT. KODE(4)) GO TO 40
         XO = XINJ(KINJ)
         TEST1=XO+3.*DELTAX
         KINJEC=1
         KPASSS=1
         SS=XO
         IF(KINJ .EQ. KODE(4)) GO TO 30
         XFIN = XINJ(KINJ +1)
         GO TO 31
      30 XFIN = XFINAL
      31 CONTINUE
         G2 =GINJ(KINJ)
         T2 =TINJ(KINJ)
         DO 32 KK = 1,NIND
      32 Y2(KK) = YINJ(KK,KINJ)
         DO 33 KK= 1,NDEP
      33 XZ2(KK) = XZINJ(KK,KINJ)
         YNO2 = YNOINJ(KINJ)
         TCOMB=TCOMBI(KINJ)
         CALL       MIX(G,Y,XZ,YNO,T,G2,Y2,XZ2,YNO2,T2,GO,YO,XZO,YNOO,TO,
        1                NIAD,NDEP,NCOMP,CPAVG,CPCOEF,IBOMB)
         IF(IBOMB.NE.0) GO TO 40
         CALL THERMO(TO,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
         CALL TADB(NINC,NDEP,NCCMP,YO,XZO,Y,XZ,DELH,DELALP,B,GAMMA,
        1           CPCCEF,CPAVG,GO,G,TO,TADAB,HEAT)
         PRINT 501, TADAB
     501 FORMAT(                              ////T20, 'ADIABATIC FLAME ',
        2       'TEMPERATURE FOR INLET GAS MIXTURE = ', F10.2, ' K',/)
         CALL       INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
        1                GAMMA,YG,XZOLD,YNOO,YNO,G,T,TB,
        2                XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
        3                DRDT,RCCN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
        4                MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
        5                TSPEC,QSPEC,KODE,GO,P,TO,XO,XFIN,DELTAX,
        6                PINT,NOPT,IBCMB,CNCHRT,QNCHTP,TCOMB,TADAB,
        7               NSPRAY,ICODE,SS,NT)
         IF(IBOMB.NE.0) GO TO 40
         GO TO 35
      50 CONTINUE
C******* CALL THE SUBROUTINE 'INTGRT' WHICH INTEGRATES THE MASS AND
C           ENERGY BALANCE EQUATICNS DOWN THE REACTCR.
         CALL       INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
        1                GAMMA,YG,XZOLD,YNOO,YNO,G,T,TB,
        2                XZG,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
        3                DRDT,RCGN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
        4                MMINV,XZ,AJACCB,FUN,XPOINT,AREA,PERIM,TWALL,
        5                TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
        6                PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TADAB,
        7               NSPRAY,ICODE,SS,NT)
         GO TO 40
         END
```

```
 0001             SUBROUTINE ADATA(NIND,NDEP,NCCMP,B,GAMMA,YO,XZO,CPCOEF,DCOF,YNOO,
                 1                CP,DCPDT,DELH,DHDT,RCON,HTC,XPOINT,AREA,PERIM,
                 2                TWALL,TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
                 3                PINT,XINJ,GINJ,TINJ,YINJ,XZINJ,YNOINJ,
                 4                NCPT,TX,CPY,C,FO,F,A,QNCHRT,QNCHTP,TCOMB,TCOMBI,
                 5                NSPRAY,ICODE,TB)
 0002             DIMENSICN B(NIND,NIND),GAMMA(NDEP,NIND),YO(NIND),XZO(NDEP)
 0003             DIMENSION CPCCEF(NCOMP,10), DCOF(NIND,14)
 0004             DIMENSION CP(NCCMP),DCPDT(NCOMP),DELH(NIND),DHDT(NIND)
 0005             CCMMON /AA/ HVAP
 0006             COMMON/P/ QCCN
 0007             COMMON/KDATA/TABLE(10,3),MODEL,NMAX1
 0008             DIMENSION PRINT(8)
 0009             DATA PRINT/
                 1  'FUEL',' OIL',' MOD','EL  ',
                 2   'COAL',' OLS','T MG','DEL '/
 0010             DIMENSION XPOINT(100),AREA(100),PERIM(100),TWALL(100)
 0011             DIMENSION QSPEC(100)
 0012             DIMENSION TSPEC(100),KCDE(NOPT)
 0013             DIMENSION HTC(3),   RCCN(10)
 0014             DIMENSION TX(20),CPY(20),C(4),FO(4),F(20,4),A(4,4)
 0015             DIMENSION XINJ(20),GINJ(20),TINJ(20),YINJ(NIND,20),XZINJ(NDEP,20)
 0016             DIMENSION YNCINJ(20)
 0017             DIMENSION QNCHRT(3), TCOMBI(20)
 0018             DIMENSION TITLE(20),ICODE(6)
 0019             DIMENSION WRITES(4,5)
 0020             COMMON/AB/R(10),RHONV(10),NGROUP,NFNCTN,RHOP,AVGMW,
                 1         VP,      WDP(10),XNDP(10)
 0021             CCMMON /EE/ FUEL
 0022             COMMON/CD/YO2EQ
 0023             COMMON /IJ/ VAPF
 0024             DATA WRITES/ 'NOT ','SPEC','IFIE','D   ','SPEC','IFIE','D   ','
                 1 ',          ' FUE','L EX','PONE','NT  ',' CO ','EXPO','NENT','
                 2 ',          'CCMP','UTED',' FRO','M QR'/
 0025             XO =      .0
 0026             B(1,2)=-0.5
 0027             B(2,2)= 1.0
 0028             GAMMA(1,2)=  0.0
 0029             GAMMA(2,2)= -1.0
 0030             GAMMA(3,2)=  0.0
 0031             GAMMA(4,2)=  0.0
 0032             READ(5,5012,END=100) (TITLE(I),I=1,20)
 0033        5012 FORMAT (20A4)
 0034             PRINT 5013,(TITLE(I),I=1,20)
 0035        5013 FORMAT (1H1,T10, 'CCMBUSTION/POLLUTION MODEL--- ',20A4 //)
 0036             READ(5,1013,END=100) KODE,NSPRAY,MODEL
 0037        1013 FORMAT(16I5)
 0038             N1 = KODE(1) + 1
 0039             N2 = KODE(2) + 1
 0040             IF (N2.EQ.3) N2=5
 0041             N3 = KODE(3) + 1
 0042             PRINT 3013, KODE(1), (WRITES(IX,N1),IX=1,4),
                 1            KCDE(2), (WRITES(IX,N2),IX=1,4),
                  2          KODE(3), (WRITES(IX,N3),IX=1,4), KODE(4)
 0043       3013 FORMAT (T1S, 'DECK 3347'
                  1      / / T16, 'INPUT SUMMARY', / T10, 26('*'), //5X, 'CARD 1 ',
                  2      '- OPTICNS', / 5X, 16('-'),//13X, I2, ' WALL TEMPERATURE ',
                  3     'PROFILE ',4A4, /13X, I2,' GAS TEMPERATURE PROFILE ', 4A4,/
                  4    13X, I2, ' HEAT FLUX PROFILE ', 4A4,/13X, I2, ' NO. OF SECON',
                  5     'DARY INJECTICN PTS.')
            C******  READ THE STOICHIGMETRIC COEFFICIENTS FOR THE FIRST REACTION.
 0044             READ(5,1000) GAMMA(1,1),B(1,1),GAMMA(2,1),GAMMA(3,1)
 0045       1000 FORMAT(7F10.3)
 0046             PRINT 3000, GAMMA(1,1), B(1,1), GAMMA(2,1), GAMMA(3,1)
 0047       3000 FORMAT (/ 5X, 'CARD 2 - STOICHICMETRIC COEFFICIENTS (FUEL COMBUS',
                 1      'TION)',/ 5X, 54('-'), // 7X, F10.3, ' FUEL COEFFICIENT',/
                 2      7X, F10.3, ' O2 COEFFICIENT ',/ 7X, F10.3,' CO COEFFICIENT',
                 3      / 7X, F1C.3,' H2O COEFFICIENT')
 0048             B(1,1) = -B(1,1)
 0049             B(2,1) = 0.0
 0050             GAMMA(1,1) = -GAMMA(1,1)
 0051             GAMMA(4,1) = C.
            C****** READ INITIAL MOLAR GAS VELOCITY,INITIAL TEMPERATURE AND
            C            PRESSURE.
 0052             READ(5,10CC) GO,TC,P,TCOMB
 0053             PRINT 3010, GC, TO, P,TCCMB
 0054        3010 FORMAT (/5X, 'CARD 3 - PHYSICAL CONDITIONS CF INLET GAS MIXTURE',
                 1      / 5X, 49('-'), // 7X, F10.3, ' FLOW RATE (G-MOLES/SEC)',/
                 2      7X, F10.3,' TEMPERATURE (K)', / 7X, F10.3,' PRESSURE(PSIA)',
                 3/7X,F10.3,' ADIABATIC FLAME TEMPERATURE AT INLET (K)')
            C******  READ THE INITIAL GAS COMPOSITION.
 0055             READ(5,100C) YC,XZO,YNOO
 0056             PRINT 3020, (YO(ID), IC=1,2), (XZO(JD), JD=1,4),YNOO
 0057        3020 FORMAT (/ 5X, 'CARD 4 - INLET GAS CCMPOSITION',/ 5X, 30('-'),//
                 1       7X, F10.3, ' MOLE FRACTION OF C2',/ 7X, F10.3, ' MOLE FRACT',
                 2       'ION CF CO2',/ 7X, F10.3, ' MOLE FRACTION OF FUEL',/ 7X,
                 3       F10.3,' MCLE FRACTION OF CO',/ 7X, F10.3, ' MOLE FRACTION',
                 4       ' OF H2O',/ 7X, F10.3, ' MOLE FRACTION OF N2 ',/ 7X, F10.3,
                 5       ' MOLE FRACTICN GF NO')
 0058             IF(KODE(4).LE.0) GC TO 5
 0059             KKKK = KODE(4)
 0060             DO 6 IK = 1,KKKK
 0061             READ(5,10C0) GINJ(IK),TINJ(IK),XINJ(IK),TOCMBI(IK)
 0062             PRINT 3030, GINJ(IK), TINJ(IK), XINJ(IK),TCOMBI(IK)
 0063        3030 FORMAT (/5X, 'CARD 5 - CONDITION AND LOCATION OF SECONCARY INJEC',
                 1       'TION GAS',/ 5X, 58('-'),// 7X, F10.3, ' FLOW RATE (G-MOLES',
                 2       '/SEC)',/ 7X, F10.3, ' TEMPERATURE(K)',/ 7X, F10.3, ' INJEC',
                 3       'TICN PCINT (FT.)',
                 4/7X,F10.3,' ADIABATIC FLAME TEMPERATURE AT INJECTION POINT (K)')
 0064             READ(5,1000)  ((YINJ(KR,IK),KR=1,NIND),(XZINJ(KR,IK),KR=1,NDEP),
                 1                 YNOINJ(IK))
 0065             PRINT 3040,  (YINJ(KR,IK), KR=1,NIND), (XZINJ(KR,IK), KR=1,NDEP),
                 1                 YNOINJ(IK)
 0066        3040 FORMAT (/5X, 'CARD 6 - INJECTICN GAS COMPOSITION',/5X, 34('-'),//
                 1       7X, F10.3, ' MOLE FRACTION OF O2',/ 7X, F10.3, ' MOLE FRACT',
                 2       'ION CF CO2',/ 7X, F10.3, ' MOLE FRACTION OF FUEL',/ 7X,
              3     F10.3, ' MGLE FRACTICN OF CO',/ 7X, F10.3, ' MOLE FRACTION',
              4     ' OF H2C',/ 7X, F10.3, ' MOLE FRACTION OF N2',/ 7X, F10.3,
              5     ' MOLE FRACTICN CF NO')
 0067           6 CONTINUE
          C****** READ IN THE CCNSTANTS IN THE FIRST RATE EXPRESSION. THE
 0068           5 READ(5,1002) RCCN
 0069        1002 FORMAT(E1C.2,4F10.3)
 0070             PRINT 3002
 0071        3002 FORMAT (/5X, 'CARD 7 - KINETIC RATE CONSTANTS FOR FUEL COMBUSTIO',
              1     'N',/5X, 51('-'),/)
 0072             PRINT 3050, (RCCN(IJ), IJ=1,4), (WRITES(IX,3), IX=1,4), RCON(5)
 0073        3050 FORMAT ( 7X, E10.2, ' FREQUENCY FACTOR',/ 7X, F10.3, ' ACTIVATIO',
              1     'N ENERGY',/ 7X, F10.3,' O2 EXPONENT',/ 7X, F10.3, 4A4,/ 7X,
              2     F10.3, ' H2O EXPGNENT')
 0074             PRINT 4002
 0075        4002 FORMAT (/5X, 'CARD 8 - KINETIC RATE CONSTANTS FOR CO COMBUSTION',
              1          /5X, 49('-'),/)
 0076             PRINT 3050, (RCCN(IJ), IJ=6,9), (WRITES(IX,4), IX=1,4), RCON(10)
 0077             IF(KODE(1) .LE. 0) GO TO 7
          C****** READ IN THE HEAT TRANSFER COEFFICIENTS.
 0078             READ(5,100C) HTC
 0079             IF (KODE(1) .EQ. 1) PRINT 3060, (HTC(IL), IL=1,3)
 0080        3060 FORMAT (/5X, 'CARD 9 - HEAT TRANSFER CONSTANTS',/5X, 32('-'),//7X,
              1     F10.3, ' CCNSTANT COEFFICIENT',/ 7X, F10.3, ' CONVECTION ',
              2     'COEFFICIENT',/ 7X, F10.3, ' RADIATION COEFFICIENT')
 0081           7 IF(KODE(2).NE.2)  GO TC 8
 0082             READ 1000, CNCHRT, QNCHTP
 0083             PRINT 4000,QNCHRT
 0084        4000 FORMAT (/5X,'CARD 9.5 - QUENCH RATE CONSTANTS',/5X,32('-'),//7X,
              1 F10.3,' FIRST COEFFICIENT'    ,/7X,F10.3,' SECOND COEFFICIENT',/
              2 7X,F10.3,' THIRD COEFFICIENT')
 0085             IF(QNCHTP.EC.0) PRINT 4001
 0086        4001 FORMAT(/7X,'QUADRATIC RATE TO BE USED')
 0087             IF(QNCHTP.EC.1) PRINT 4003
 0088        4003 FORMAT(/7X,'EXPCNENTIAL RATE TO BE USED')
 0089           8 CONTINUE
 0090             KK = 0
 0091             PRINT 1014
 0092        1014 FORMAT (/5X, 'CARD 10 - CCMBUSTOR PROFILES',/5X, 28('-'),//
              1          10X,'DISTANCE   CROSS-SECTIONAL AREA   PERIMETER   WALL TE
              1MPERATURE   GAS TEMPERATURE      HEAT FLUX',/11X,'(FEET)',12X,
              2'(FT2)',12X,'(FEET)',11X,'(K)',15X,'(K)',9X,'(KCAL/FT2-SEC)'/
              3 11X,6('-'),12X,5('-'),12X,6('-'),11X,3('-'),15X,3('-'),9X,14('-')
              5//)
 0093          20 KK = KK+1
 0094             READ(5,1012)XPOINT(KK),AREA(KK),PERIM(KK),TWALL(KK),TSPEC(KK),
              1QSPEC(KK),KCHECK
 0095        1012 FORMAT(6F1C.3,19X,I1)
 0096             PRINT 3012, XPOINT(KK), AREA(KK), PERIM(KK), TWALL(KK), TSPEC(KK),
              1     QSPEC(KK)
 0097        3012 FORMAT(8X,F10.3,8X,F10.3,8X,F10.3,5X,F10.3,8X,F10.3,9X,F10.3)
 0098             IF(KCHECK.LE.0) GO TO 20
          C******  READ IN REACTOR LENGTH AND PRINT INTERVAL.
```

```
0099             READ(5,1000) XFINAL,PINT,DELTAX
0100             PRINT 3070, XFINAL, PINT,DELTAX
0101        3070 FORMAT (/5X, 'CARD 11 - COMBUSTOR LENGTH AND PRINOUT INTERVAL',/
               1         5X, 47('-'),// 7X, F10.3, ' REACTOR LENGTH (FEET)',/ 7X,
               2         F1C.3, ' PRINTCUT INTERVAL (FEET)',
               3 /7X,F10.3,'INTEGRATION INTERVAL (FEET)')
0102             TREF = 298.
           C****    READ THE HEATS OF REACTION AT THE REFERENCE TEMPERATURE.
0103             READ(5,1000) (DCOF(IR,11),IR = 1,NIND)
0104             PRINT 3080, (DCCF(IR,11), IR= 1,NIND)
0105        3080 FORMAT (/5X, 'CARD 12 - HEAT OF REACTION AT 298K',/ 5X, 34('-'),//
               1     7X, F10.3, ' HEAT OF REACTION FOR FUEL COMBUSTION',/ 7X,
               2     F10.3, ' HEAT OF REACTION FOR CO COMBUSTION')
           C     READ IN THE HEAT CAPACITY DATA FOR FUEL AND CURVE FIT IT.
           C     WRITE(6,1010)
           C1010 FORMAT(1H1,'HEAT CAPACITY DATA FOR   FUEL      IS FITTED BY THE FO
           C    1LLOWING FUNCTION,'//,' FOR T .GE. 298K AND .LE. 1200K',/,' CP= A1
           C    2+ A2*(T/1000.) + A3*(T/1000.)**2 + A4*(T/1000.)**3 + A5*(T/1000.)*
           C    3*4',//,' FOR T .GT. 1200K',/,' CP= A6 + A7/(T/1000.) + A8/((T/1000
           C    4.)**2) + A5/((T/1000.)**3) + A10/((T/1000.)**4)',////)
0106             KASE = 0
0107             NCON = 4
0108             READ(5,2000)NPTS,TI,CPI
0109             PRINT 3090, NPTS, TI, CPI
0110        3090 FORMAT (/5X, 'CARD 13 - HEAT CAPACITY DATA FOR FUEL (298K TO 1200K
               1)',       / 5X, 53('-'), // 13X, I2,' NO. OF HEAT CAPACITY DATA',
               2           ' PCINTS FOR FUEL (298K TO 1200K)', // 5X, 'CARD 14 - HE',
               3          'AT CAPACITY DATA POINTS FOR FUEL (298K TO 1200K)', / 5X,
               4           60('-'),//7X, 'TEMPERATURE (K)', 4X, 'HEAT CAPACITY OF FU'
               5          ,'EL (CAL/G-MCLES, K)',/7X, 15('-'), 4X, 37('-'),//10X,
               6           F10.3, 20X, F10.3)
0111             NPTS = NPTS - 1
0112        2000 FORMAT(I4,/,4X,2F10.3)
0113             CALL        CPFIT(NPTS,NCON,TI,CPI,TX,CPY.CO,C,FO,F,A,KASE)
           C     WRITE(6,20C2)CO,C
           C2002 FORMAT(1H ,'CCEFFICIENTS IN THE HEAT CAPACITY EQUATION FOR T L.E.
           C    11200K ARE,',//,8X,'A1',14X,'A2', 14X,'A3',14X,'A4',14X,'A5',/(5E16
           C    2.4)//////////)
0114             CPCOEF(3,1) = CO
0115             DO 18 KC = 1,4
0116             KCC = KC + 1
0117          18 CPCOEF(3,KCC) = C(KC)
0118             KASE = 1
0119             TI = 1200.
0120             TR = 1.
0121             CPI = CO
0122             DO 1 KK= 1,NCCN
0123             TR  = TR *1.2
0124           1 CPI = CPI+ C(KK)*TR
0125             READ(5,1001) NPTS
0126        1001 FORMAT(I4)
0127             PRINT 3110, NPTS
0128        3110 FORMAT (/5X, 'CARD 15 - HEAT CAPACITY DATA FOR FUEL (T > 1200K)',
     1        /5X, 48('-'),//13X, I2, ' NO. OF HEAT CAPACITY DATA ',
     2        'PCINTS FOR FUEL (T > 1200K)',// 5X, 'CARD 16 - HEAT CAP',
     3        'ACITY DATA PCINTS FOR FUEL (T > 1200K)',/5X,54('-'),//7X,
     4       'TEMPERATURE (K)', 4X, 'HEAT CAPACITY OF FUEL (CAL/G-MOLE',
     5        'S,K)',/7X, 15('-'), 4X, 37('-'),/)
      CALL      CPFIT(NPTS,NCON,TI,CPI,TX,CPY,CO,C,FO,F,A,KASE)
      CPCOEF(3,6) = CO
      DO 19 KC = 1,4
      KCC = KC + 6
   19 CPCOEF(3,KCC) = C(KC)
C     WRITE(6,1004)CO,C
C1004 FORMAT(1H ,'COEFFICIENTS IN THE HEAT CAPACITY EQUATION FOR T G.E.
C    11200K ARE,',//,8X,'A6',14X,'A7', 14X,'A8',14X,'A9',14X,'A10',/(5E1
C    26.4))
C**** CALCULATE THE CCEFFICIENTS IN THE DELTA CP EXPRESSION.
      DO 10 IREAT = 1,NIND
      DO 10 IC = 1,10
      DCOF(IREAT,IC) = 0.
      DO 9 IR = 1,NIND
    9 DCOF(IREAT,IC) = DCOF(IREAT,IC) + B(IR,IREAT)*CPCOEF(IR,IC)
      DO 10 IR=1,NDEP
      NC = IR + NIND
   10 DCOF(IREAT,IC) = DCOF(IREAT,IC) + GAMMA(IR,IREAT)*CPCOEF(NC,IC)
C****    CALCULATE THE ADDITIONAL CCNSTANTS NEEDED
      TR = TREF/1000.
      T1 = 1.
      DO 11  IR = 1,NIND
   11 DCOF(IR,13) = 0.
      DO 12 IC =1,5
      AC = IC
      T1 = T1*TR
      T2= T1/AC
      DO 12 IR =1,NIND
   12 DCOF(IR,13) = DCOF(IR,13) + DCOF(IR,IC) *T2
      DO 13 IR=1,NIND
   13 DCOF(IR,14) = 0.
      DO 14 IR = 1,NIND
   14 DCOF(IR,14) = DCOF(IR,6)*1.2
      T2 = ALOG(1.2)
      DO 15 IR = 1,NIND
   15 DCOF(IR,14) = DCOF(IR,14) + DCOF(IR,7)*T2
      T2 = 1.
      T1 = 1.0
      DO 16 IC = 8,10
      AC = IC - 7
      T1= T1/1.2
      T2= T1/AC
      DO 16 IR = 1,NIND
   16 DCOF(IR,14) = DCOF(IR,14) - DCOF(IR,IC)*T2
      T1 = 1.2
      T2 = T1*1.2
      T3 = T2*1.2
      T4 = T3*1.2
```

```
 0171              T5 = T4*1.2
 0172              DO 17 IR = 1,NIND
 0173           17 DCOF(IR,12) = DCOF(IR,11) +       (DCOF(IR,1)*T1 + DCOF(IR,2)*T2/
                  12. + DCOF(IR,3)*T3/3. + DCOF(IR,4)*T4/4. + DCOF(IR,5)*T5/5. -
                  2 DCOF(IR,13))
 0174              READ 90,YO2EQ,QCCN
 0175           90 FORMAT(5E1C.4)
 0176              PRINT 94,QCCN
 0177           94 FORMAT(//12X,'THE QUENCH RATE IS IMPOSED AT ',F4.2,' OF THE ADIABA
                  1TIC FLAME TEMPERATURE'///)
         C         QCON=QUENCH CCNSTANT
 0178              IF(YO2EQ.LE.0.)GO TO 93
 0179              PRINT 91,YO2EQ
 0180           91 FORMAT(//// 12X,'THE EQUILIBRIUM MOLE FRACTION OF O2 IS ASSUMED TO
                  1 BE=',E10.4)
 0181           93 IF(NSPRAY.EQ.0)      RETURN
 0182              READ 25,(ICODE(I),I=1,NCCMP),NFNCTN,NGROUP,RHOP,AVGMW,FUEL,TB,
                  1      VAPF,HVAP
 0183           25 FORMAT(6I2,2I3,4F10.1,2E10.1)
 0184              N=NSPRAY
 0185              IF (NSPRAY .EQ. 2) N=5
 0186              NIX = N + 3
 0187              PRINT 6000,(PRINT(IX), IX = N, NIX),  NGROUP,AVGMW,RHOP,TB,VAPF,
                  1            HVAP
 0188         6000 FORMAT (/5X, 'CARD 18 - ', 4A4, / 5X, 25('-'),
                 1        // 12X, I3, ' PARTICLE SIZE DISTRIBUTION',
                 2        / 5X, F10.1, ' MOLECULAR WEIGHT OF FUEL IN VAPOR STATE',
                 3        / 5X, F10.1, ' DENSITY OF FUEL OIL DROPLETS',
                 4        / 5X, F10.1, ' BOILING POINT OF FUEL OIL (OK)',
                 5        / 5X, E10.1, ' VAPORIZATION CONSTANT (FT**2/SEC)',
                 6        / 5X, E10.1, ' HEAT OF VAPORIZATION (CAL/GM-MOLE)')
 0189              DO 22 I=1,NGRCUP
 0190              READ 21,R(I),WDP(I)
 0191           21 FORMAT(2E10.1)
 0192           22 CONTINUE
 0193              RETURN
 0194          100 STOP
 0195              END
```

```
      SUBROUTINE INTGRT(NIND,NDEP,NDIM,NCOMP,DABINV,YO,YOLD,Y,GAMBIV,B,
     1                  GAMMA,YG,XZOLD,YNOD,YNC,G,T,TB,
     2                  XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
     3                  DRDT,RCON,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
     4                  MMINV,XZ,AJACOB,FUN,XPOINT,AREA,PERIM,TWALL,
     5                  TSPEC,QSPEC,KODE,GO,P,TO,XO,XFINAL,DELTAX,
     6                 PINT,NOPT,IBOMB,QNCHRT,QNCHTP,TCOMB,TACAB,
     7                 NSPRAY,ICODE,SS,NT)
      DIMENSION DABINV(NIND),YG(NIND),Y(NIND),YOLD(NIND),YO(NIND)
      DIMENSION GAMBIV(NDEP,NIND),XZOLD(NDEP)
      DIMENSION B(NIND,NIND), XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
      DIMENSION DCOF(NIND,14)
      DIMENSION DGIDY(NIND),DXZDY(NDEP,NIND),R(NIND),DRDY(NIND,NIND)
      DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
      DIMENSION DGCPDY(NIND),DELH(NIND),DHDT(NIND),LMINV(NDIM)
      DIMENSION MMINV(NDIM)
      DIMENSION XZ(NDEP),AJACOB(NDIM,NDIM),FUN(NDIM)
      DIMENSION XPOINT(100),AREA(100),PERIM(100),TWALL(100)
      DIMENSION TSPEC(100),KODE(NOPT)
      DIMENSION QSPEC(100)
      DIMENSION QNCHRT(3)
      DIMENSION GAMMA(NDEP,NIND)
      DIMENSION HTC(3),    RCON(10)
      DIMENSION XMOLE( 6),ICODE( 6),XZ2(4),Y2(2),CPAVG(6)
      DIMENSION YTEMP(2), XZTEMP(4)
      DIMENSION YFUEL(2),XFUEL(4)
      COMMON /EE/ FUEL
      COMMON/P/ QCON
C
C
C*************************************************************
C*                                                           *
C*    THIS SUBROUTINE IS THE EXECUTIVE PROGRAM FOR THE FIRST *
C*    ORDER IMPLICIT INTEGRATION ROUTINE.  IT IS MAINLY CON- *
C*    CERNED WITH SELECTING THE INITIAL CONDITIONS FOR THE   *
C*    ITERATIVE SCHEME AND CHOOSING THE PROPER STEP SIZE.    *
C*                                                           *
C*************************************************************
C
C
      KPRINT=0
      YNOEQ = 0.
C
C         CALL OUTONE TO PRINT HEADINGS
C
      IF(NSPRAY.NE.0)GO TO 138
      CALL OUTONE(NEND,NDEP,X,G,Y,XZ,YNC,T,1,YNOEQ)
  138 ACCUR=1.E-4
      MAXITR=50
      KSTOP=0
      XPRINT=XO
      X=XO
      STEP=DELTAX
```

```
FORTRAN IV G LEVEL  19                  INTGRT                                                         PAGE 0002
                C
                C*****WHEN FUEL IS LICUID CR SOLID WE MUST COMPUTE
                C      THE AMOUNT EVAPCRATED OR GASIFIED.
 0032                  IF(NSPRAY.EQ.0)GO TO 140
 0033                  IF(SS.NE.0.)GO TO 140
 0034                  A=AREA(1)
                C
                C*********SUBROUTINE SPRAY CCMPUTES THE AMOUNT OF LIQUID
                C            OR SOLID FUEL VAPORIZED OR GASIFIED
                C
 0035                 CALL SPRAY(A,STEP,RATES,NT,NSPRAY,TB,TO,P,GO)
 0036                 IF(NSPRAY.EQ.0)NSPRAY=3
                C
                C*********PROCEED TC CALCULATE A NEW COMPOSITION AND
                C            TEMPERATURE BY MIXING THE GAS STREAM WITH
                C            THE EVAPORATED FUEL.--THESE CCMPUTATIONS
                C            ARE PERFORMED BY SUBROUTINE UPCATE.
                C
 0037                YNOO=0.
 0038                YNO2=0.
 0039                TI=TO
 0040                CALL UPDATE(GO,YO,XZO,YNOO,TO,RATES,TB,G2,Y2,XZ2,YNO2,T2,NIND,
                    1           NDEP,NCOMP,CPAVG,CPCOEF,IBOMB,SS,TI)
 0041                CALL THERMO(T2,NIND,NCCMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
               C
               C           CALCULATE ADIABATIC FLAME TEMPERATURE FOR ALL THE FUEL
               C
 0042                G3=GO + FUEL
 0043                NTOTAL=NIND+NDEP
 0044                DO 49 I=1,NTOTAL
 0045                IF (ICODE(I) .EQ. 1) GO TO 47
 0046                IF (I .GT. NIND) GO TO 46
 0047                YTEMP(I)=GO*YO(I)/G3
 0048                GO TO 49
 0049             46 II = I-NIND
 0050                XZTEMP(II)=GO*XZO(II)/G3
 0051                GO TO 49
 0052             47 IF (I .GT. NIND) GO TO 48
 0053                YTEMP(I)=FUEL/G3
 0054                GO TO 49
 0055             48 II = I-NIND
 0056                XZTEMP(II) = FUEL/G3
 0057             49 CONTINUE
 0058                CALL TADB(NIND,NDEP,NCCMP,YTEMP,XZTEMP,Y,XZ,DELH,DELALP,
                   1  B,GAMMA,CFCOEF,CPAVG,G3,G,T2,TADAB,HEAT)
 0059                PRINT 499,TADAB
 0060            499 FORMAT(1H1,58X,'CCMBUSTICN/POLUTION MODEL',//64X,'OUTPUT',
                   1      ' SUMMARY',//57X,19('*'),////T20,'ADIABATIC FLAME ',
                   2      'TEMPERATURE OF VAPORIZED LIQUID/SOLID FUEL = ',F10.2,' K',
                   3      /)
              C
              C         CALL OUTCNE TO PRINT HEADINGS
              C
```

```
0061              TO=T2
0062              CALL OUTCNE(NIND,NDEP,X,G,Y,XZ,YNO,T,1,YNOEQ)
0063              CALL OUTCNE(NIND,NDEP,X,GO,YO,XZO,YNOO,TO,2,YNOEQ)
            C
            C
            C---------RE-INITIALIZE
            C
            C
0064              DO 118 I=1,NIND
0065          118 YO(I)=Y2(I)
0066              DO 119 I=1,NDEP
0067          119 XZO(I)=XZ2(I)
0068              YNOO=YNO2
0069              TO=T2
0070              GO=G2
0071          140 G=GO
0072              T=TO
0073              YNO=YNOO
0074              YNOEQ=0.
0075              DO 1 II = 1,NIND
0076              YO(II) = YO(II)
0077              YOLD(II)= YO(II)
0078            1 Y(II) = YO(II)
0079              DO 2 II = 1,NDEP
0080              XZOLD(II) = XZO(II)
0081            2 XZ(II) = XZO(II)
0082              IF(NSPRAY.NE.0)GO TO 142
0083              CALL OUTCNE(NIND,NDEP,X,G,Y,XZ,YNO,T,2,YNOEQ)
0084          142 KOUNT=0
0085              XOLD= XO
0086              TOLD= TO
0087              GOLD= GO
0088              YNOLD= YNOO
0089              KOOK=0
0090              IF(NSPRAY.NE.0)GO TO 311
            C
            C     IF SPRAY IS LIQUID OR SOLID GO TO 311
            C     TO CHECK FOR FUEL AVAILABILITY.
            C
            C
            C**** CHECK FOR OXYGEN AVAILABILITY
            C
            C
            C     ASSUME,AS AN INITIAL GUESS IN THE NEWTON-RAPHSON,
            C     THAT 50 PERCENT OF OXYGEN REACTS WITH THE FUEL.
            C
0091              Y(1) = .5*YO(1)
            C
            C         CALCULATE THE NUMBER OF MOLES OF O2 CONSUMED,Y1R1,
            C         IF ALL THE FUEL BURNS TO CO .
            C
0092              Y1R1= (B(1,1)/GAMMA(1,1))*XZO(1)
            C
            C         CHECK IF ENOUGH GXYGEN IS AVAILABLE TO BURN
            C         ALL THE FUEL
            C
 0093             IF(YO(1).GT.Y1R1) GO TO 300
 0094             Y2ADD=-.00001
 0095             GO TO 310
            C
            C     IF THERE IS ENOUGH OXYGEN TO AT LEAST BURN
            C     FUEL TO CO, CHECK HOW PUCH OF THE CO CAN BE
            C     BURNED TO CO2 WITH REMAINING OXYGEN.
            C
            C     XZ2R1=NUMBER CF MOLES CF CO PRODUCED PER MOLE OF FEED
            C     XZO(2)=MOLE FRACTICN OF CO
            C     GAMMA(2,1)=STCCHICMETRIC COEFFICIENT OF CO IN REACTION 1.
            C     GAMMA(1,1)=STCCHICMETRIC COEFFICIENT OF FUEL IN REACTION 1.
            C     XZO(1)=MOLE FRACTION OF GASEOUS FUEL IN THE FEED
            C     B(1,2)=STOCHICMETRIC COEFFICIENT OF OXYGEN IN REACTION 2.
            C
            C     REACTION 1=  FUEL + OXYGEN= CO + H2O
            C     REACTION 2=  CC + OXYGEN= CO2
            C
 0096         300 XZ2R1=XZO(2)-(GAMMA(2,1)/GAMMA(1,1))*XZO(1)
            C
            C     XZ2R1=NUMBER CF MOLES CO AVAILABLE FROM REACTION 1
            C           PLUS THAT INITIALLY PRESENT IN THE INLET GAS.
            C
            C     Y1R2=MOLES CF C2 CCNSUMED BY OXIDATION OF CO.
            C
 0097             Y1R2=(B(1,2)/GAMMA(2,2))*XZ2R1
            C
            C     IF THE OXYGEN AVAILABLE IS NOT SUFFICIENT TO
            C     BURN ALL THE CO TO CO2,GO TO 320 AND COMPUTE
            C     HOW MUCH CO2 CAN BE PRCDUCED WITH O2 THAT'S LEFT.
            C
 0098             IF(YO(1).LT.(Y1R1+Y1R2)) GO TO 320
            C
 0099             Y2ADD=(GAMPA(2,1)/GAMMA(1,1))*XZO(1)
            C     Y2ADD=MOLES OF CO  THAT CAN BE OXIDIZED TO CO2
            C           IF THERE IS ENOUGH OXYGEN TO BURN ALL THE
            C           FUEL TO CO2.
            C
 0100             GO TO 310
            C
 0101         320 Y2ADD=(B(2,2)/B(1,2))*(YO(1)-Y1R1)
            C
            C           THE ABCVE CALCULATICN REFLECTS THAT
            C           ONLY A PORTICN OF THE CO CAN BE BURNED
            C           TO CO2 FOR LACK CF OXYGEN.
            C
 0102         310 Y(2)=YO(2)-C.49990*Y2ADD
 0103             GO TO 325
            C
            C
```

```
          C**** CHECK FOR GAS-FUEL AVAILABILITY IF FUEL IS
          C     INJECTED IN THE LIQUID OR SOLID STATE.
          C
          C         COMPUTE THE AMCUNT OF CC THAT CAN BE PRODUCED.
          C         WITH AVAILABLE GASEOUS FUEL.
          C
 0104       311 Y1R1=B(1,1)/GAMMA(1,1)*XZO(1)
          C
          C     Y1R1=AMCUNT OF GXYGEA CONSUMED BY OXIDATION
          C           OF AVAILABLE FUEL TO CO.
          C
          C     IF THERE IS ENOUGH OXYGEN TO BURN TO CO,PROCEED
          C     TO CALCULATE HOW MUCH CO CAN BE BURNED TO CO2
 0105           IF(YO(1).GT.Y1R1)GO TO 312
          C
          C
          C     IF THERE IS NOT EAOUGH GXYGEN TO PRODUCE CO2
          C     I WANT AT LEAST TO PRODUCE A TINY FRACTION OF IT.
 0106           Y2ADD=-0.0C001
 0107           GO TO 324
          C
          C         COMPUTE THE AMCUNT OF CO PRODUCED IF
          C         REACTICN 1 GOES TO CCMPLETICN AND ADD
          C         TO CO ENTERING WITH THE FUEL.
          C
 0108       312 XZ2R1=XZO(2)- GAMMA(2,1)/GAMMA(1,1)*XZO(1)
          C
          C     Y1R2=AMOUNT OF CXYGEN CCASUMED BY REACTION 2
          C
 0109           Y1R2=(B(1,2)/GAMMA(2,2))*XZ2R1
 0110           IF(YO(1).LT.(Y1R1+Y1R2))GO TO 313
 0111           Y2ADD=GAMMA(2,1)/GAMMA(1,1)*XZO(1)
 0112           GO TO 324
 0113       313 Y2ADD=(B(2,2)/B(1,2))*(YO(1)-Y1R1)
 0114       324 Y(2)=YO(2)-0.49990*Y2ADD
 0115           Y(1)=YO(1)-C.5*(Y1R1+Y1R2)
 0116           Y(1)=YO(1)*C.5
 0117       325 KOOK=0
 0118           T=TADAB*0.93
 0119           IF(NSPRAY.GT.0)T=2000.
 0120           TTO = T
 0121        51 IF (DELTAX.EQ.0.0) DELTAX = (XFINAL-XO)/128.
 0122           IF(PINT.LT.DELTAX) DELTAX=PINT
 0123           XPRINT = XPRINT + PINT
 0124           IF(KODE(2).NE.2.OR.TCCMB.NE.0.) GO TO 330
 0125           KODE(1) = 2
 0126           KODE(2)=0
 0127           DELTX = DELTAX
 0128           XPRINT =XO+DELTAX
 0129           DO 65 II= 1,3
 0130        65 HTC(II) = 0.0
 0131           GO TO 330
          C
```

```
      C
      C******* CALCULATE THE NEXT PRINT POSITICN.
      C
      C
          9 IF((XFINAL-XPRINT) .GT. (PINT +DELTAX)) GO TO 3
            XPRINT = XFINAL
            KSTOP =  1
            GO TO 4
          3 XPRINT = XPRINT + PINT
      C
      C
      C
      C
      C**** GET READY TO TAKE ANCTHER INTEGRATION STEP
      C
      C
      C
          4 IF(NSPRAY.EQ.0)GO TO 44
            CALL SPRAY(A,STEP,RATES,NT,NSPRAY,TB,T,P,G)
            CALL UPDATE(G,Y,XZ,YNC,T,RATES,TB,G2,Y2,XZ2,YNO2,T2,NIND,NDEP,
           1            NCOMP,CPAVG,CPCOEF,IBCMB,SS,TI)
      C
      C
            DO 41 I=1,NIND
            YO(I)=Y2(I)
         41 YO(I)=Y2(I)
            DO 42 I=1,NDEP
            XZO(I)=XZ2(I)
         42 XZ(I)=XZ2(I)
            YNOO=YNO2
            YNO=YNO2
            TO=T2
            T=T2
            G=G2
            GO=G2
         44 DO 5 II=1,NIND
            YOLD(II) = YO(II)
          5 Y(II) = YO(II)
            DO 22 II = 1,NDEP
         22 XZOLD(II) = XZ(II)
            XOLD = X
            TOLD = T
            GOLD = G
            YNOLD = YNC
      C******* CHOOSE THE NEXT INTEGRATION STEP LENGTH.
        330 IF((XPRINT-XOLD).GE. (2.*DELTAX))  GO TO 6
            IF((XPRINT-XCLD).LE.(1.0001*DELTAX   )) GO TO 7
            STEP = .5*(XPRINT - XGLD)
            GO TO 8
          6 STEP = DELTAX
            GO TO 8
          7 STEP = XPRINT - XCLD
            KPRINT = 1
      8 X = XOLD + STEP
        KPOINT=1
        GO TO 21
     20 KPOINT = KPCINT + 1
        KO = KPOINT-1
     21 IF( X.GT.XPCINT(KPCINT)) GO TO 20
        THTA=(X - XPCINT(KO))/(XPOINT(KPOINT) - XPCINT(KO))
        A = AREA(KC)+ THTA*(AREA(KPOINT) - AREA(KO))
        S = PERIM(KO)+ THTA*(PERIM(KPOINT) -PERIM(KO))
        IF(KODE(1) .LE. 0) GC TO 60
        TW = TWALL(KO) + THTA*(TWALL(KPOINT)-TWALL(KO))
        GO TO 62
     60 IF(KODE(2) .LE. 0) GO TO 61
        IF(KODE(2).EQ.2) GO TC 63
        TS = TSPEC(KC) + THTA*(TSPEC(KPOINT) - TSPEC(KO))
        GO TO 62
     63 CALL QUENCH(TCOMB,X,XOLD,GCLD,P,A,QNCHRT,QNCHTP,TS)
        TCOMB = TS
        GO TO 62
     61 QTRAN = QSPEC(KC) + THTA*(QSPEC(KPOINT) - QSPEC(KO))
     62 CONTINUE
C******* CALL 'SCLVE' THE SUBROUTINE WHICH SOLVES ,VIA. A NEWTON -
C           RAPHSON METHOD- THE SET OF NONLINEAR ALGEBRAIC EQUATIONS
C           RESULTING FRGM THE FIRST ORDER IMPLICIT  FINITE DIFFERENCE
C           SCHEME USED TO INTEGRATE THE DIFFERENTIAL  EQUATIONS
        CALL        SCLVE(NIND,NDEP,NDIM,NCCMP,DABINV,YO,YOLD,Y,GAMBIV,B,
       1                  YC,TTC,GAMMA,XZOLD,
       2                  XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
       3                  DRDT,RCCN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
       4                  MMINV,XZ,AJACOB,FUN,KODE,GO,Q,P,T,TOLD,TW,TS,
       5                  QTRAN,A,S,STEP,ACCUR,Y1MIN,MAXITR,KCESS,NOPT,
       6                  IBOMB,NSPRAY)
        IF(IBOMB.NE.0) RETURN
        IF(KCESS .LT. 0) GO TO 111
        CALL POLUT(P,T,GGLD,G,YNCLD,STEP,A,XZ(4),Y(1),YNO,YNOEQ,SS)
        IF(NSPRAY.EQ.3)NSPRAY=0
        SS=SS+STEP
    100 IF(KPRINT .GT. 0) GO TC 50
        IF(KODE(1).NE.2) GO TO 4
        IF(T.LT.(QCON*TADAB).AND.ABS(T-TOLD).GT.01)GO TO 4
        XPRINT=X
        GO TO 50
     50 CALL OUTONE(NIND,NDEP,X,G,Y,XZ,YNO,T,2,YNOEQ)
        IF(X.GE.XFINAL)RETURN
        IF(KSTOP .GT. 0) GC TO 500
        KPRINT = 0
        IF ( KODE(1).NE.2) GC TO 9
        IF(T.LT.(QCON*TADAB).AND.ABS(T-TOLD).GT.01)GO TO 9
        KODE(1) = 0
        KODE(2) = 2
        DELTAX = DELTX
        TCOMB = T
        GO TO 9
```

```
FORTRAN IV G LEVEL  19                  INTGRT
                                                                              PAGE 0008
 0212          111 WRITE(6,1001)
 0213         1001 FORMAT(1H1,'THE NEWTCN-RAPHSON ITERATION IN SOLVE HAS FAILED TO
                  1CONVERGE.  CURRENT VALUES OF INTEREST ARE AS FOLLOWS.')
 0214              CALL OUTCNE(KIND,NDEP,X,G,Y,XZ,ANCX,T,2,YNDEQ)
 0215              IBOMB=1
 0216          500 RETURN
 0217         1010 CONTINUE
 0218         1011 CONTINUE
 0219              IBOMB=1
 0220              RETURN
 0221              END
```

```
FORTRAN IV G LEVEL  19                 JACOB                                                  PAGE 0001

            SUBROUTINE JACOB(NIND,NDEP,NDIM,NCOMP,DABINV,YO,Y,GAMBIV,B,XZO,
           1                   YC,TTC,GAMMA,XZOLD,STEP,
           2                   DELALP,CPCOEF,DCOF, DGIDY,DXZDY,R,DRDY,DRDXZ,
           3                   DRDT,RCCN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,XZ,
           4                   AJACOB,FUN,KODE,GO,P,T,TW,TS,QTRAN,A,S,G,NOPT,
           5 IBCMB)
            DIMENSION DABINV(NIND),YO(NIND),Y(NIND),GAMBIV(NDEP,NIND)
            DIMENSION B(NIND,NIND), XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
            DIMENSICN DCOF(NIND,14),YO(NIND),GAMMA(NDEP,NIND),XZOLC(NDEP)
            DIMENSION DGIDY(NIND),CXZDY(NCEP,NIND),R(NIND),DRDY(NIND,NIND)
            DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
            DIMENSICN DGCPDY(NIND),DELH(NIND),DHDT(NINC)
            DIMENSICN XZ(NDEP),AJACOB(NDIM,NDIM),FUN(NDIM)
            DIMENSICN KODE(NOPT)
            DIMENSION HTC(3),   RCCN(10)
            MAXTIM = 1CO
            MAX = 0
         28 MAX = MAX + 1
            IF(MAX .GT. MAXTIM) GC TO 30
      C
      C ***    CALCULATE THE TOTAL MOLAR FLOW RATE OF GAS,G,AND THE DERIVATIVE
      C          W.R.T. THE INDEPENDENT CCMPOSITION VARIABLES.
      C
            ANUM = 1.
            DENCM=1.
            DO 1 KK =1,NIND
            ANUM= ANUM - CABINV(KK)*YO(KK)
          1 DENOM = DENOM - DABINV(KK)*Y(KK)
            G = GO*ANUM/DENCM
      C
      C
      C******** CALCULATE THE PARTIAL OF  1./G  W.R.T. THE INDE-
      C         PENDENT COMPCNENTS Y(I).  THIS IS STORED IN DGIDY.
      C
      C
            DO 2 KK = 1,NIND
          2 DGIDY(KK) = - DABINV(KK)/(GO*ANUM)
      C
      C***  CALCULATE THE DEPENDENT CCMPCSITIONS AND THEIR DERIVATIVES W.R.T.
      C       THE INDEPENDENT COMPCSITICNS.
      C
            GOBYG = GO/G
            DO 4 KK = 1,NDEP
            T1 = 0.
            T2 = 0.
      C
      C******** CALCULATE THE CONCENTRATICNS OF THE DEPENDENT COMPCNENTS
      C
            DO 3 JJ = 1,NIND
            T1 = T1 + GAMBIV(KK,JJ)*Y(JJ)
          3 T2 = T2 + GAMBIV(KK,JJ)*YO(JJ)
            XZ(KK) = GOBYG*(XZO(KK)-T2) + T1
      C
```

```
FORTRAN IV G LEVEL  19                JACOB                                       PAGE 0002
          C******** CALCULATE THE PARTIAL OF XZ,DXZDY,W.R.T. Y .
          C
                DO 4 LL=1,NIND
              4 DXZDY(KK,LL)=DGIDY(LL)*GO*XZO(KK)+GAMBIV(KK,LL)- DGIDY(LL)*GO*T2
                DO 25 KK = 1,NDEP
          C
          C           CHECK FOR NEGATIVE VALUES OF XZ(DEPENDENT COMPONENTS)
          C
                IF(XZ(KK).LE.0.C) GO TC 26
             25 CONTINUE
                GO TO 30
             26 AMU = 0.5
                DO 27 KK = 1,NIND
             27 Y(KK) = (1.-AMU)*YO(KK) + AMU*Y(KK)
                GO TO 28
             30 IF((XZ(1) .GT. .0001) .AND. (XZ(2) .GT. .0001))GO TO 31
                A1= RCON(1)
                E1= RCON(2)
                C11=RCON(3)
                C12=RCON(4)
                C13=RCON(5)
                C10 = C11+C12+C13
                CA= P/(14.7*.C8205)
                A1 = A1*28.32*(CA**C10)
                CA1= EXP(-E1/(1.987*T))
                C1= A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(3)**C13)
                IF(XZOLD(1).LT.1.E-40) GO TO 33
                IF(XZ(1) .GT. .0001) GC TO 34
                XZ1S=XZ(1)
                XZ(1) = -((G*XZOLD(1))/(A*GAMMA(1,1)*STEP))/C1
                IF(XZ(1).LE.1.E-9)XZ(1)=1.E-9
                XZ(1) = XZ(1)**(1./C12)
                IF(XZ1S.LT.XZ(1).AND.XZ1S.GT.0.0) XZ(1)=XZ1S
                GO TO 34
             33 XZ(1) = XZCLD(1)
             34 IF(XZOLD(2).LT.1.E-40.AND.XZOLD(2).NE.0.0) GO TO 35
                IF(XZ(2) .GT. .0001) GO TO 31
                A2=RCON(6)
                E2=RCON(7)
                C21=RCON(8)
                C22=RCON(9)
                C23=RCON(1C)
                C20=C21+C22+C23
                A2 =A2*28.32*(CA**C20)
                CA2=EXP(-E2/(1.987*T))
                C2=A2*CA2*( (1./T)**C20)*(Y(1)**C21)*(XZ(3)**C23)
                R(1)= C1*(XZ(1)**C12)
                XZ2S=XZ(2)
                XZ(2) =-((G*XZCLD(2))/(A*STEP) + GAMMA(2,1)*R(1))/(GAMMA(2,2)*C2)
                XZ(2) =  XZ(2)**(1./C22)
                IF(XZ2S.LT.XZ(2).AND.XZ2S.GT.0.0) XZ(2)=XZ2S
                GO TO 31
             35 XZ(2) = XZCLD(2)
```

```
FORTRAN IV G LEVEL  19                  JACOB                                             PAGE 0003
                C********CALCULATE THE FUNCTIONS ON THE RIGHT HAND SIDE OF THE NDIM
                C         DIFFERENTIAL EQUATIONS AND ALSO THE JACOBIAN MATRIX
                C         CORRESPONDING TO THESE FUNCTIONS.
 0079              31 CONTINUE
                C
                C
                C******** CALL SUBROUTINE RATE TO CALCULATE DRDXZ AND DRDT
                C           WHICH ARE THE DERIVATIVES OF THE SPECIFIC REACTION
                C           VELOCITY, OF EACH OF THE COMBUSTION REACTIONS,
                C           WITH RESPECT TO XZ AND T.
                C
                C
 0080                 CALL       RATE(NIND,NDEP,Y,XZ,P,T,RCON,R,DRDY,DRDXZ,DRDT)
                C
                C******** CALCULATE DRDY WHICH IS THE DERIVATIVE OF THE SPE-
                C           CIFIC REACTION VELOCITY WITH RESPECT TO Y.
                C
 0081                 DO 6 II = 1,NIND
 0082                 DO 6 JJ = 1,NIND
 0083                 T1 = 0.
 0084                 DO 5 KK = 1,NDEP
 0085               5 T1 = T1 + DRDXZ(II,KK)*DXZDY(KK,JJ)
 0086               6 DRDY(II,JJ) =  DRDY(II,JJ)+T1
 0087                 DO 7 II = 1,NDIM
 0088                 DO 7 JJ = 1,NDIM
 0089               7 AJACOB(II,JJ) = 0.
 0090                 T0 = 0.
 0091                 DO 8 II = 1,NIND
                C
                C       THE FOLLOWING STATEMENTS DOWN TO AND INCLUDING STATEMENT 12
                C         CALCULATE THE FIRST NIND FUNCTIONS AND THE PARTIAL DERIVATIVES
                C         OF THESE FUNCTIONS W.R.T. THE INDEPENDENT COMPOSITION VARIABLES
                C         AND THE TEMPERATURE.
                C
 0092               8 T0 = T0 - DELALP(II)*R(II)
 0093                 T0 = A*T0/G
 0094                 DO 12 LL = 1,NIND
 0095                 T1 = 0.
 0096                 T2 = 0.
 0097                 DO 10 JJ = 1,NIND
 0098                 C1 = B(LL,JJ) - Y(LL)*DELALP(JJ)
 0099                 T1 = T1+ C1*R(JJ)
 0100                 T2 = T2 + C1*DRDT(JJ)
 0101                 DO 10 MM = 1,NIND
 0102              10 AJACOB(LL,MM) = AJACOB(LL,MM) + C1*DRDY(JJ,MM)
 0103                 DO 11 MM = 1,NIND
 0104                 AJACOB(LL,MM) = A*AJACOB(LL,MM)/G + A*DGIDY(MM)*T1
 0105                 IF(MM.EQ.LL) AJACOB(LL,MM) = AJACOB(LL,MM)+T0
 0106              11 CONTINUE
 0107                 AJACOB(LL,NDIM) = A*T2/G
 0108              12 FUN(LL) = A*T1/G
 0109                 IF(KODE(2) .GT. 0)GO TO  21
                C
```

```
      C********CALCULATE THE FUNCTION ON THE R.H.S. OF THE TEMP. D.E. AND
      C         THE PARTIAL DERIVATIVES OF THIS FUNCTION W.R.T. THE INDEPENDENT
      C         COMPOSITION VARIABLES AND TEMPERATURE.
      C
            CALL       THERMO(T,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
        990 CONTINUE
            T1=0.
            T2=0.
            T3=0.
            DO 13 LL = 1,NIND
            T1 = T1 + Y(LL)*CP(LL)
         13 T2 = T2 + Y(LL)*DCPDT(LL)
            DO 14 LL = 1, NDEP
            LPNIND = LL + NIND
            T1 = T1+XZ(LL)*CP(LPNIND)
         14 T2 = T2+XZ(LL)*DCPDT(LPNIND)
            DO 16 LL = 1,NIND
            DGCPDY(LL) = CP(LL)
            DO 15 KK=1,NDEP
            KPNIND = KK + NIND
         15 DGCPDY(LL) = DGCPDY(LL) + CP(KPNIND)*DXZDY(KK,LL)
         16 DGCPDY(LL) = (-DGCPDY(LL)/(G*T1) + DGIDY(LL))/T1
            DGCPDT = - T2/(G*T1*T1)
            DO 17 JJ = 1, NIND
         17 T3 = T3 -DELH(JJ)*R(JJ)
            CALL       HLOSS(T,TW,QTRAN,HTC,QLOSS,DQLDT,KODE,NOPT)
            T3 = A*T3-S*QLOSS
            FUN(NDIM) = T3/(G*T1)
            DO 19 KK = 1,NIND
            AJACOB(NDIM,KK) = 0.
            DO 18 JJ = 1,NIND
         18 AJACOB(NDIM,KK) = AJACOB(NDIM,KK) - DELH(JJ)*DRDY(JJ,KK)
         19 AJACOB(NDIM,KK) = AJACOB(NDIM,KK) * A/(G*T1) + DGCPDY(KK)*T3
            DO 20 JJ = 1,NIND
         20 AJACOB(NDIM,NDIM) = AJACOB(NDIM,NDIM) - DELH(JJ)*DRDT(JJ)-DHDT(JJ)
           1*R(JJ)
            AJACOB(NDIM,NDIM)=(AJACOB(NDIM,NDIM)*A - S*DQLDT)/(G*T1) + DGCPDT
           1*T3
       9990 CONTINUE
            RETURN
         21 DO 22 LL = 1,NDIM
         22 AJACOB(NDIM,LL) = 0.
            RETURN
       1000 WRITE(6,1001)
       1001 FORMAT(1H ,'A FEASIBLE SOLUTION CANNOT BE FOUND....JACOB')
            IBOMB=1
            RETURN
            END
```

```
                                                                                PAGE 0001
FORTRAN IV G LEVEL  19                  SCLVE
 0001            SUBROUTINE SOLVE(NIND,NDEP,NDIM,NCCMP,DABINV,YO,YOLD,Y,GAMBIV,B,
               1                    YC,TTC,GAMMA,XZOLD,
               2                    XZO,DELALP,CPCOEF,DCOF,DGIDY,DXZDY,R,DRDY,DRDXZ,
               3                    DRDT,RCCN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,LMINV,
               4                    MMINV,XZ,AJACOB,FUN,KODE,GO,G,P,T,TOLD,TW,TS,
               5                    CTRAN,A,S,STEP,ACCUR,Y1MIN,MAXITR,KCESS,NOPT,
               6                   IBOMB,NSPRAY)
 0002            DIMENSION DABINV(NIND),YO(NIND),Y(NIND),YOLD(NIND),YO(NIND)
 0003            DIMENSION GAMBIV(NDEP,NIND),GAMMA(NDEP,NIND),XZOLD(NDEP)
 0004            DIMENSION B(NIND,NIND), XZO(NDEP),DELALP(NIND),CPCOEF(NCOMP,10)
 0005            DIMENSION DCCF(NIND,14)
 0006            DIMENSION DGIDY(NIND),DXZDY(NDEP,NIND),R(NIND),DRDY(NIND,NIND)
 0007            DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND),CP(NCOMP),DCPDT(NCOMP)
 0008            DIMENSICN DGCPDY(NIND),CELH(NIND),DHDT(NINC),LMINV(NDIM)
 0009            DIMENSION MMINV(NDIM)
 0010            DIMENSION XZ(NDEP),AJACOB(NCIM,NDIM),FUN(NDIM)
 0011            DIMENSION HTC(3),   RCCN(10)
 0012            DIMENSICN KODE(NOPT)
 0013            DIMENSICN YSAVE(2)
           C
           C*****************************************************************
           C*                                                               *
           C*    THIS SUBROUTINE SETS UP AND SOLVES BY NEWTCN-RAPHSON THE   *
           C*    EQUATIONS FOR THE FIRST ORDER IMPLICIT FINITE DIFFERENCE   *
           C*    SCHEME. IT USES SUBRCUTINE JACOB TO COMPUTE THE JACOBIAN.  *
           C*                                                               *
           C*****************************************************************
           C
           C
 0014            IDBUG=1
 0015            ITER=0
           C
           C
           C          IF GAS TEMPERATURE PROFILE IS NOT SPECIFIED GO TO 30
           C
 0016            IF(KODE(2).LE.0)GO TC 30
 0017            T=TS
 0018            TTO=T
 0019         30 CONTINUE
 0020        100 ITER=ITER + 1
 0021            IF(ITER.GT.MAXITR) GO TO 300
 0022            DO 50 KK=1,NIND
 0023         50 YSAVE(KK)=Y(KK)
 0024            CALL        JACOB(NIND,NDEP,NDIM,NCCMP,DABINV,YO,Y,GAMBIV,B,XZO,
               1                    YO,TTO,GAMMA,XZOLD,STEP,
               2      DELALP,CPCOEF,DCCF ,DGIDY,DXZDY,R,DRDY,DRDXZ,
               3                    DRDT,RCCN,CP,DCPDT,DGCPDY,DELH,DHDT,HTC,XZ,
               4                    AJACOB,FUN,KODE,GO,P,T,TW,TS,QTRAN,A,S,G,NOPT,
               5 IBOMB)
 0025            IF(IBOMB.NE.0) RETURN
 0026            ICONV=0
 0027            DO 51 KK=1,NIND
 0028            IF(Y(KK).EQ.YSAVE(KK).CR.ABS((Y(KK)-YO(KK))/YO(KK)).GE..001.OR.
                 1 ITER.EQ.1) GO TO 52
 0029           51 CONTINUE
 0030              ICONV=1
 0031           52 CONTINUE
              C
              C-------- AS CCNVERGENCE IS ACHIEVED FUN(NDIM) APPROACHES ZERO
              C
 0032              DO 1 II=1,NIND
 0033            1 FUN(II)= Y(II)-STEP*FUN(II)- YOLD(II)
 0034              IF(KODE(2) .GT. 0) GO TO 6
              C
              C------- IF KODE(2) = 1, GAS TEMPERATURE PROFILE IS SPECIFIED.
              C
 0035              FUN(NDIM)= T  -STEP*FUN(NDIM)-TOLD
 0036              GO TO 7
              C
              C          WHEN GAS TEMPERATURE PROFILE IS SPECIFIED,
              C          FUN(NDIM) BECOMES ZERO SINCE T=TS.
              C
 0037            6 FUN(NDIM)=T-TS
 0038            7 CONTINUE
              C
              C
              C********AFTER THE CALL TG JACOB, THE MATRIX AJACOB CONTAINS THE
              C          PARTIAL DERIVATIVES OF FUN W.R.T. THE INDEPENDENT COMPOSITION
              C          VARIABLES.  THE FOLLOWING STATEMENTS DOWN TO AND INCLUDING
              C          STATEMENT 3 CALCULATE THE JACOBIAN CORRESPONDING TO THE FIRST
              C          ORDER IMPLICIT SCHEME USED HERE.
              C
              C
 0039              DO 3 II = 1,NDIM
 0040              DO 3 JJ = 1,NDIM
 0041              AJACOB(II,JJ) = -STEP*AJACOB(II,JJ)
 0042              IF(II.EQ.JJ) AJACOB(II,JJ)= 1. + AJACOB(II,JJ)
 0043            3 CONTINUE
 0044              CALL MINV(AJACOB,NDIM,D,LMINV,MMINV)
 0045              TTO = T
 0046              DO 4 KK = 1,NIND
 0047              YO(KK) = Y(KK)
 0048              IF(KK.EQ.2) GO TO 41
 0049              IF(YOLD(KK).LT.1.E-40) GO TO 43
 0050              IF(Y(KK).LT.1.0E-20) GO TO 4
 0051              GO TO 42
 0052           43 Y(KK)=YOLD(KK)
 0053              GO TO 4
 0054           41 IF(YOLD(KK).GE.1.E-40.OR.YOLD(KK).EQ.0.0) GO TO 42
 0055              GO TO 43
 0056           42 DO 40 JJ=1,NDIM
 0057           40 Y(KK)= Y(KK)- AJACOB(KK,JJ)*FUN(JJ)
 0058            4 CONTINUE
 0059           12 DO 5  JJ = 1,NDIM
 0060            5 T = T- AJACOB(NDIM,JJ)*FUN(JJ)
 0061          130 IF(T.GT.TTO)GO TO 133
```

```
          RATIO=T/TTO
          CHECK=C.S5
          IF(RATIC.LT.CHECK)T=TTG*CHECK
             GO TO 134
      133 RATIO=T/TTC
          CHECK=1.05
          IF(RATIO.GT.CHECK) T=TTO*CHECK
      134 IF(Y(1).LE.O..CR.Y(2).LE.O.) GO TO 15
          ADIST = ABS((T-TTO)/100.)
          DO 13 KK = i,NIND
          HOLD =(ABS (Y(KK) - YC(KK)))/YO(KK)
          IF(HOLD .GT. ADIST) ADIST = HCLD
       13 CONTINUE
          IF(ADIST .LT. .CO1  ) GO TO 200
          ANCRM = 0.
          DO 2 II = 1,NDIM
        2 ANORM = ANGRM + FUN(II)*FUN(II)
          ANORM = SQRT(ANCRM)
          IF(ANORM .LT. ACCUR) GO TO 200
          IF(ABS((T-TTC)/100.).GE..001) GO TO 15
          IF(ICONV.EG.0) GO TO 15
          GO TO 200
       15 MAX = C
       11 MAX = MAX + 1
          IF(MAX .GT. 1C) GC TO 20
          IF(Y(1).LE.O.C.CR.Y(2).LE.O.O) GO TC 9
          GO TO 14
        9 AMU = .50
          DO 10 KK = 1,NIND
       10 Y(KK) = (1. - AMU)*YO(KK) + AMU*Y(KK)
          GO TO 11
       14 CONTINUE
          GO TO 100
      200 KCESS = +1
C         T = TTO
C         DO 17 KK = 1,NIND
C      17 Y(KK) = YO(KK)
C         GO TO 400
          RETURN
      300 KCESS = -1
      400 RETLRN
       20 WRITE(6,1000)
     1000 FORMAT(1HO,'A FEASIBLE SOLUTION CAN NOT BE FOUND .....SOLVE')
          IBOMB=1
          RETURN
          END
```

```
FORTRAN IV G LEVEL  19                 TACB                                                   PAGE 0001

 0001             SUBROUTINE  TADB(NIND,NDEP,NCCMP,YO,XZO,Y,XZ,DELH,DELALP,B,GAMMA,
                 1                     CPCOEF,CPAVG,GO,G,TO,TACAB,HEAT)
 0002             DIMENSION YO(NIND),Y(NIND),XZO(NDEP),XZ(NDEP),DELALP(NIND)
 0003             DIMENSION DELH(NIND),B(NIND,NIND),GAMMA(NDEP,NIND)
 0004             DIMENSION CPCCEF(NCOMP,10),CPAVG(NCOMP)
            C 990 CONTINUE
 0005             IF(YO(1) .GT.  (B(1,1)/GAMMA(1,1))*XZO(1)) GO TO 50
            C     THERE IS  LESS C2 THAN REQUIRED TO CARRY THE FIRST REACTION TO
            C     COMPLETION. CCNSICER TFE FIRST REACTION COMPLETELY DOMINATES.
            C     THE HEAT RELEASED IS (IT IS POSITIVE)
 0006             HEAT =(GO*YO(1))* (DELH(1)/B(1,1))
 0007             G = GO*(1. - (DELALP(1)/B(1,1))*YO(1))
 0008             Y(1) = 0.
 0009             Y(2) =(GO/G)*(YO(2) - B(2,1)/  B(1,1)*YO(1))
 0010             DO 1 KK = 1,NDEP
 0011           1 XZ(KK) =(GO/G)*(XZO(KKT -  GAMMA(KK,1)/B(1,1)*YO(1))
 0012             GO TO 100
 0013          50 CONTINUE
            C     THERE IS MORE THAN ENOUGH OXYGEN TO CARRY THE FIRST REACTION TO
            C     COMPLETION.
 0014             G = GO*(1. - (DELALP(1)/GAMMA(1,1))*XZO(1))
            C     THE HEAT RELEASED BY THE FIRST REACTION GOING TO COMPLETION IS,
 0015             HEAT =(GO*XZO(1))*DELH(1)/GAMMA(1,1)
 0016             DO 2 KK = 1,NIND
 0017           2 Y(KK) = (GO/G)*(YO(KK) - B(KK,1)/GAMMA(1,1) * XZO(1))
 0018             DO 3 KK = 1,NDEP
 0019           3 XZ(KK) = (GO/G)*(XZO(KK) -GAMMA(KK,1)/GAMMA(1,1) *XZO(1))
            C     IS THERE ENOUGH O2 TC COMPLETELY CONVERTE THE CO FORMED BY THE
            C     FIRST REACTION.
 0020             IF(Y(1) .GT.  B(1,2)/GAMMA(2,2)*XZ(2)) GO TO 75
            C     THERE IS NOT ENOUGH O2 TO TAKE THE SECOND REACTION TO COMPLETION.
            C     THE HEAT RELEASED IS.
 0021             HEAT = HEAT + G*Y(1)*DELH(2)/B(1,2)
 0022             G1= G
 0023             G =G1*(1. - DELALP(2)/B(1,2) *Y(1))
 0024             Y(2)=(G1/G)*(Y(2) - B(2,2)/B(1,2)*Y(1))
 0025             DO 4 KK = 1,NDEP
 0026           4 XZ(KK) =(G1/G)*(XZ(KK)- GAMMA(KK,2)/B(1,2)*Y(1))
 0027             Y(1) = 0.
 0028             GO TO 100
 0029          75 CONTINUE
            C     THERE IS ENOUGH O2 TO CARRY SECOND REACTION TO COMPLETION.
            C     THE HEAT RELEASED BY THE SECOND REACTION IS.
 0030             HEAT = HEAT + G*XZ(2)*DELH(2)/GAMMA(2,2)
 0031             G1= G
 0032             G =G1*(1. - DELALP(2)/GAMMA(2,2)*XZ(2))
 0033             DO 5 KK = 1,NIND
 0034           5 Y(KK) =(G1/G)*(Y(KK) - B(KK,2)/GAMMA(2,2) * XZ(2))
 0035             DO 6 KK = 1,NDEP
 0036             IF(KK.EQ. 2) GO TO  6
 0037             XZ(KK) =(G1/G)*(XZ(KK) - GAMMA(KK,2)/GAMMA(2,2) * XZ(2))
 0038           6 CONTINUE
 0039             XZ(2) = 0.
```

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FORTRAN IV G LEVEL  19                 TACB                                                   PAGE 0002
 0040              100 CONTINUE
 0041                  TL = TO
 0042                  TH = 3000.
 0043                  FL =-HEAT
 0044                  CALL  CAVG(NCCMP,CPCCEF,CPAVG,TO,TH)
 0045                  A1= 0.
 0046                  DO 11 KK= 1,NIND
 0047               11 A1 = A1+Y(KK)*CPAVG(KK)
 0048                  DO 12 KK= 1,NDEP
 0049                  KKP= KK+NIND
 0050               12 A1 = A1+XZ(KK)*CPAVG(KKP)
 0051                  FH = -HEAT + G*A1*(TH-TO)
 0052                  IF(FH .LT. 0.) GO TO 5000
 0053                  KOUNT = 0
 0054                  TM=0.0
 0055               30 KOUNT =KOUNT +1
 0056                  IF(KOUNT .GT.50) GO TO 5001
 0057                  TMS=TM
 0058                  TM =(TL*FH - TH*FL)/(FH-FL)
 0059                  CALL  CAVG(NCOMF,CPCOEF,CPAVG,TO,TM)
 0060                  A1 = 0.
 0061                  DO 13 KK = 1,NIND
 0062               13 A1 = A1 + Y(KK)*CPAVG(KK)
 0063                  DO 14 KK = 1,NDEP
 0064                  KKP=KK+NIND
 0065               14 A1 =A1 + XZ(KK)*CPAVG(KKP)
 0066                  FM = -HEAT + G*A1*(TM-TO)
 0067                  IF(ABS(TM-TMS).LT..01) GO TO 22
 0068                  IF(FM .LT. 0.) GC TO 23
 0069                  FH = FM
 0070                  TH = TM
 0071                  GO TO 30
 0072               23 FL =FM
 0073                  TL =TM
 0074                  GO TO 30
 0075               22 TADAB = TM
                C9990 CONTINUE
 0076                  RETURN
 0077             5000 WRITE(6,1111)
 0078             1111 FORMAT(1H0,'THE ADIABATIC FLAME TEMP. IS GT 3000.K')
 0079                  TADAB=3100.
 0080                  RETURN
 0081             5001 WRITE(6,1112)
 0082             1112 FORMAT(1H ,'THE ADIABATIC FLAME TEMP. WAS NCT LOCATED.')
 0083                  TADAB=0.0
 0084                  RETURN
                C      DEBUG INIT , TRACE
                C      AT 990
                C      TRACE ON
                C      AT 9990
                C      TRACE OFF
 0085                  END
```

```
FORTRAN IV G LEVEL  19                    RATE                                        PAGE 0001

 0001              SUBROUTINE RATE(NIND,NDEP,Y,XZ,P,T,RCON,R,DRDY,DRDXZ,DRDT)
 0002              DIMENSION Y(NIND),XZ(NDEP),RCON(10),DRDY(NIND,NIND),R(NIND)
 0003              DIMENSION DRDXZ(NIND,NDEP),DRDT(NIND)
            C***   RATE EXPRESSIONS SUPPLIED BY THE USER ARE OF THE FORM
            C      A. FOR FUEL GOING TO CO AND H2O
            C      R(1)= A1*EXP(-E1/(1.987*T))*((O2)**C11)*((FUEL)**C12)*((H2O)**C13)
            C      B. FOR CO GOING TO CO2.
            C      R(2)= A2*EXP(-E2/(1.987*T))*((O2)**C21)*((CO)**C22)*((H2O)**C23)
            C      THE UNITS HERE ARE,
            C      R , MOLES/(LITER-SEC.)
            C      E1,E2,   CAL./MOLE
            C      T        , DEGREE KELVIN
            C      (COMP.), MOLES/LITER
            C      THE CONSTANTS A1,A2,.....,C23 ARE IN THE ARRAY RCON
 0004              A1 = RCON(1)
 0005              E1 = RCON(2)
 0006              C11= RCON(3)
 0007              C12= RCON(4)
 0008              C13= RCON(5)
 0009              A2 = RCON(6)
 0010              E2 = RCON(7)
 0011              C21= RCON(8)
 0012              C22= RCON(9)
 0013              C23= RCON(10)
 0014              C10 = C11+C12+C13
 0015              C20 = C21+C22+C23
            C      CONVERT THE RATE EXPRESSIONS TO THE UNITS OF MOLES/((CUBIC FT.)*(SEC.))
            C      BY MULTIPLYING BY 28.32 LITERS/CUBIC FOOT. AT THE SAME TIME CONVERT
            C      TO MOLE FRACTIONS.
 0016              CA = P/(14.7*.08205)
 0017              A1 = A1*28.32*(CA**C10)
 0018              A2 = A2*28.32*(CA**C20)
 0019              CA1 = EXP(-E1/(1.987*T))
 0020              CA2 = EXP(-E2/(1.987*T))
 0021              R(1) = A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(1)**C12)*(XZ(3)**C13)
 0022              R(2) = A2*CA2*((1./T)**C20)*(Y(1)**C21)*(XZ(2)**C22)*(XZ(3)**C23)
 0023              DRDY(1,1) = C11*A1*CA1*((1./T)**C10)*(Y(1)**(C11-1.))*(XZ(1)**C12)
                  1            *(XZ(3)**C13)
 0024              DRDY(1,2) = 0.
 0025              DRDY(2,1) = C21*A2*CA2*((1./T)**C20)*(Y(1)**(C21-1.))*(XZ(2)**C22)
                  1            *(XZ(3)**C23)
 0026              DRDY(2,2) = 0.
 0027              DRDXZ(1,1)= C12*A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(1)**(C12-1.))
                  1            *(XZ(3)**C13)
 0028              DRDXZ(1,2)=0.
 0029              DRDXZ(1,3)= C13*A1*CA1*((1./T)**C10)*(Y(1)**C11)*(XZ(1)**C12)
                  1            *(XZ(3)**(C13-1.))
 0030              DRDXZ(1,4)= 0.
 0031              DRDXZ(2,1) =0.
 0032              DRDXZ(2,2)= C22*A2*CA2*((1./T)**C20)*(Y(1)**C21)*(XZ(2)**(C22-1.))
                  1            *(XZ(3)**C23)
 0033              DRDXZ(2,3)= C23*A2*CA2*((1./T)**C20)*(Y(1)**C21)*(XZ(2)**C22)
                  1            *(XZ(3)**(C23-1.))
```

```
FORTRAN IV G LEVEL  19                RATE                                    PAGE 0002

 0034              DRDXZ(2,4)= C.
 0035              DRDT(1) =  R(1)*(E1/(1.987*T*T) - C10/T)
 0036              DRDT(2) =  R(2)*(E2/(1.987*T*T) - C20/T)
 0037              RETURN
 0038              END
```

```
FORTRAN IV G LEVEL  19                 HLCSS                                                    PAGE 0001

            SUBROUTINE HLOSS(T,TW,QTRAN,HTC,QLOSS,DQLDT,KODE,NOPT)
            DIMENSION KODE(NCPT)
            DIMENSION HTC(3)
            IF(KODE(3).GT.0) GO TO 1
            QLOSS = HTC(1) + HTC(2)*(T-TW) + HTC(3)*(T**4 - TW**4)
            DQLDT = HTC(2) + 4.*HTC(3)*T**3
            RETURN
          1  QLOSS = QTRAN
            DQLDT = 0.
            RETURN
            END
```

```
FORTRAN IV G LEVEL  19                OUTONE                                    PAGE 0001

                SUBROUTINE OUTONE(NIND,NDEP,X,G,Y,XZ, YNO,T,KASE,YNOEQ)
                DIMENSION Y(NIND),XZ(NDEP)
                IF(KASE .LT. 2) GO TO 1
                WRITE(6,1000)X,G,T,Y,XZ,YNO,YNOEQ
           1000 FORMAT (1H0,G11.4,10G12.4)
                GO TO 10
              1 WRITE(6,1001)
           1001 FORMAT(//2X,'DISTANCE',4X,'FLOW RATE',7X,'T',10X,'O2',10X,'CO2',
               1 8X,'FUEL',9X,'CO',10X,'H2O',9X,'N2',10X,'NO',8X,'NO(EQ)',/4X,
               2 '(FT)',4X,'(G-MOLS/SEC)',5X,'(K)',9X,36('-'),'(MOLE FRACTION)',
               3 37('-'))
             10 RETURN
                END
```

```
FORTRAN IV G LEVEL  19              CAVG                                        PAGE 0001
      SUBROUTINE CAVG(NCCMP,CPCOEF,CPAVG,T1,T2)
      DIMENSION CPCCEF(NCOMP,10) , CPAVG(NCOMP)
      DO 10 KK =1,NCCMP
   10 CPAVG(KK) = C.
      U1= T1/1000.
      H1 = U1
      U2= T2/100C.
      IF(U1.LT. 1.2) GO TO 1
      H2 = U2
      GO TO 50
    1 IF(U2.LE. 1.2) GO TO 2
      H2= 1.2
      GO TO 3
    2 H2 = U2
    3 CONTINUE
      V1=1.
      V2=1.
      DO 4 KK =1,5
      AK= KK
      V1= V1*H1
      V2= V2*H2
      DO 5 KPN = 1,NCCMP
      CPAVG(KPN)= CPAVG(KPN)+CPCOEF(KPN,KK)*(V2 - V1)/AK
    5 CONTINUE
    4 CONTINUE
      IF(U2 .LE. 1.2) GC TC 75
      H2= U2
      H1= 1.2
   50 DO 6 KPN =1,NCCMP
      CPAVG(KPN)= CPAVG(KPN)+CPCOEF(KPN,6)*(H2-H1)+CPCOEF(KPN,7)*ALOG(H
     12/H1)
    6 CONTINUE
      AK = 0.
      V1 = 1.
      V2 = 1.
      DO 7 KK =8,10
      AK= AK+1.
      V1= V1/H1
      V2= V2/H2
      DO 8 KPN =1,NCOMP
      CPAVG(KPN) =CPAVG(KPN) -(1./AK)*CPCOEF(KPN,KK)*(V2 - V1)
    8 CONTINUE
    7 CONTINUE
   75 DO 76 KPN = 1,NCCMP
   76 CPAVG(KPN)=CPAVG(KFN)/(T2 - T1)
      RETURN
      END
```

```
FORTRAN IV G LEVEL  19                CPFIT                                                PAGE 0001
           SUBROUTINE  CPFIT(NPTS,NCON,TO,CPO,TX,CPY,CO,C,FO,F,A,KASE)
           DIMENSION TX(NPTS),CPY(NPTS),C(NCON),FO(NCON),F(NPTS,NCON)
           DIMENSION A(NCON,NCON)
           DO 25  II = 1,NPTS
           READ(5,2000) TX(II),CPY(II)
           PRINT 125, TX(II), CPY(II)
       125 FORMAT (10X, F10.3, 20X, F10.3)
        25 CONTINUE
      2000 FORMAT(4X,2F10.3)
           TO = TO/1000.
           DO 100 II =1,NPTS
       100 TX(II)= TX(II)/1000.
         1 IF(KASE.GT.0) GO TO 2
           Z= TO
           GO TO 3
         2 Z = 1./TO
         3 FO(1) = Z
           DO 4 II=2,NCON
           IM1 =II-1
         4 FO(II) = FO(IM1)*Z
           DO 5 II = 1,NPTS
           IF(KASE.GT.0) GO TO 6
           Z = TX(II)
           GO TO 7
         6 Z= 1./TX(II)
         7 F(II,1)= Z
           DO 8 KK= 2,NCON
           KKM1 = KK-1
         8 F(II,KK) = F(II,KKM1)*Z
           DO 5 KK= 1,NCON
         5 F(II,KK) = F(II,KK)-FO(KK)
           DO 11 KK = 1,NCON
           DO 11 II = 1,NCON
           A(KK,II) = 0.
           DO 11 JJ = 1,NPTS
        11 A(KK,II) = A(KK,II)+ F(JJ,KK)*F(JJ,II)
           DO 12 KK = 1,NCON
           C(KK)=0.
           DO 12 JJ= 1,NPTS
        12 C(KK)= C(KK)+ F(JJ,KK)*(CPY(JJ)-CPO)
           CALL SIMQ(A,C,NCON,KS)
           IF(KS.LT.1 ) GO TO 15
           WRITE(6,1000)
      1000 FORMAT(' A SINGULAR SET OF EQUATION HAS BEEN ENCOUNTERED')
           GO TO 17
        15 CO = CPO
           DO 16 II = 1,NCON
        16 CO = CO- C(II)*FO(II)
        17 RETURN
           END
```

```
FORTRAN IV G LEVEL  19                MIX
0001              SUBROUTINE MIX(G1,Y1,XZ1,YNO1,T1,G2,Y2,XZ2,YNO2,T2,G3,Y3,XZ3,YNO3,   PAGE 0001
                 1                T3,NIND,NDEP,NCCMP,CPAVG,CPCOEF,IBOMB)
0002              DIMENSION Y1(NIND),XZ1(NDEP),Y2(NIND),XZ2(NDEP),Y3(NIND),XZ3(NDEP)
0003              DIMENSION CPCOEF(NCOMP,10),CPAVG(NCOMP)
            C 990 CONTINUE
            C     DO MATERIAL BALANCES
0004              G3= G1+G2
0005              DO 1 KK = 1,NIND
0006            1 Y3(KK) = (G1*Y1(KK) + G2*Y2(KK))/G3
0007              DO 2 KK = 1,NDEP
0008            2 XZ3(KK) = (G1*XZ1(KK) + G2*XZ2(KK))/G3
0009              YNO3 = (G1*YNO1 + G2*YNO2) / G3
            C     DO ENERGY BALANCE
            C     THE REFERENCE TEMP. IS 298K
0010              TR=298.
0011              IF(T1.EQ.T2) GO TO 25
0012              CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,T1)
0013              A1 = 0.
0014              B1 = 0.
0015              DO 3 KK=1,NIND
0016              B1 = B1 + Y3(KK)*CPAVG(KK)
0017            3 A1 = A1 + Y1(KK)*CPAVG(KK)
0018              DO 4 KK=1,NDEP
0019              KKP = KK + NIND
0020              B1 = B1 + XZ3(KK)*CPAVG(KKP)
0021            4 A1 = A1 + XZ1(KK)*CPAVG(KKP)
0022              H1 = G1*A1*(T1-TR)
0023              CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,T2)
0024              A2 =0.
0025              B2 =0.
0026              DO 5 KK=1,NIND
0027              A2 = A2 + Y2(KK)*CPAVG(KK)
0028            5 B2 = B2 + Y3(KK)*CPAVG(KK)
0029              DO 6 KK=1,NDEP
0030              KKP = KK+NIND
0031              B2  =B2 + XZ3(KK)*CPAVG(KKP)
0032            6 A2 = A2 + XZ2(KK)*CPAVG(KKP)
0033              H2 = G2*A2*(T2-TR)
0034              F1 = G3*B1*(T1-TR)-H1-H2
0035              F2 = G3*B2*(T2-TR)-H1-H2
0036              IF(T1 .GT. T2) GO TO 7
0037              TL =T1
0038              FL =F1
0039              TH =T2
0040              FH =F2
0041              GO TO 8
0042            7 TL=T2
0043              FL=F2
0044              TH=T1
0045              FH=F1
0046            8 KOUNT =0
0047              TM=0.0
0048           99 KOUNT =KOUNT + 1
```

```
          IF(KOUNT.GT.50) GC TO 234
          TMS=TM
          TM = (TL*FH - TH*FL)/(FH-FL)
          AM = 0.
          CALL CAVG(NCCMP,CPCOEF,CPAVG,TR,TM)
          DO 9 KK = 1,NIND
        9 AM = AM + Y3(KK)*CPAVG(KK)
          DO 10 KK =1,NDEP
          KKP = KK+NIND
       10 AM  = AM + XZ3(KK)*CFAVG(KKP)
          FM = G3*AM*(TM-TR)-H1-H2
          IF(ABS(TM-TMS).LT..01) GO TO 100
          IF (FM .LT. C.) GO TO 11
          FH = FM
          TH = TM
          GO TO 99
       11 FL = FM
          TL = TM
          GO TO 99
      100 T3 = TM
          RETURN
       25 T3 = T1
          RETURN
      234 WRITE(6,1000)
    C9990 CONTINUE
     1000 FORMAT(' A SCLUTICN CAN NOT BE FOUND......MIX')
          IBOMB=1
          RETURN
    C     DEBUG INIT,TRACE
    C     AT 990
    C     TRACE ON
    C     AT 9990
    C     TRACE OFF
          END
```

```
FORTRAN IV G LEVEL  19              THERMO                                    PAGE 0001

          SUBROUTINE THERMO(T,NIND,NCOMP,CPCOEF,DCOF,CP,DCPDT,DELH,DHDT)
          DIMENSICN CPCOEF(NCGMP,10),DCOF(NIND,14),CP(NCOMP)
          DIMENSION DCPDT(NCCMP),DELH(NIND),DHDT(NIND)
          TR = T/100C.
          IF(T .GT. 1200.) GO TG 100
          TR2 = TR *TR
          TR3= TR2*TR
          TR4= TR3*TR
          TR5= TR4*TR
          DO 1  II =1,NCCMP
          CP(II)=(CPCOEF(II,1) + CPCOEF(II,2)*TR + CPCOEF(II,3)*TR2
         1        +CPCCEF(II,4)*TR3 + CPCOEF(II,5)*TR4)/1000.
        1 DCPDT(II)=(CPCOEF(II,2)+2.*CPCOEF(II,3)*TR +3.*CPCOEF(II,4)*TR2
         1            +4.*CPCGEF(II,5)*TR3)/(1000.*1000.)
          DO 2 II = 1,NIND
          DHDT(II)=(DCOF(II,1) +GCOF(II,2)*TR + DCOF(II,3)*TR2
         1          +DCOF(II,4)*TR3 + DCOF(II,5)*TR4)/1000.
        2 DELH(II) =DCOF(II,11)+         (DCOF(II,1)*TR + DCOF(II,2)*TR2/2.
         1+ DCOF(II,3)*TR3/3. + DCOF(II,4)*TR4/4.  + DCOF(II,5)*TR5/5.
         2- DCOF(II,13))
          RETURN
      100 TR1 = 1./TR
          TR2 = TR1/TR
          TR3 = TR2/TR
          TR4 = TR3/TR
          DO 4 II = 1,NCCMP
          CP(II) =(CPCOEF(II,6) + CPCOEF(II,7)*TR1 + CPCOEF(II,8)*TR2
         1          + CPCOEF(II,9)*TR3 + CPCOEF(II,10)*TR4)/1000.
        4 DCPDT(II) = -(CPCOEF(II,7) + 2.*CPCOEF(II,8)*TR1 + 3.*CPCOEF(II,9)
         1              *TR2 + 4.*CPCOEF(II,10)*TR3)/(1000.*1000.*TR2)
          DO 5 II = 1,NIND
          DHDT(II) =(DCOF(II,6) + DCOF(II,7)*TR1 + DCOF(II,8)*TR2
         1          +DCOF(II,9)*TR3 + DCOF(II,10)*TR4)/1000.
        5 DELH(II) = DCOF(II,12) +          ( DCOF(II,6)*TR + DCOF(II,7)*
         1          ALOG(TR) - DCOF(II,8)*TR1 - DCOF (II,9)*TR2/2.
         2            - DCOF(II,10)*TR3/3. - DCOF(II,14) )
          RETURN
          END
```

```
FORTRAN IV G LEVEL  19                BINVER                                                  PAGE 0001

 0001               SUBROUTINE BINVER(NIND,B,BINV)
 0002               DIMENSION B(NIND,NIND),BINV(NIND,NIND)
 0003               D = B(1,1)*B(2,2) - B(1,2)*B(2,1)
 0004               BINV(1,1)= B(2,2)/D
 0005               BINV(1,2)= -B(1,2)/D
 0006               BINV(2,1)= -B(2,1)/D
 0007               BINV(2,2)= B(1,1)/D
 0008               RETURN
 0009               END
```

```
FORTRAN IV G LEVEL  19                QUENCH                                              PAGE 0001

            SUBROUTINE QUENCH(TCOMB,X,XOLD,GCLD,P,A,GNCHRT,QNCHTP,TS)
            DIMENSION GNCHRT(3)
            IF(QNCHTP.EQ.1.) GO TO 10
            TRATE=QNCHRT(1)+QNCHRT(2)*TCOMB+QNCHRT(3)*TCOMB*TCOMB
            GO TO 20
         10 TRATE= (QNCHRT(1)+ GNCHRT(2)*TCOMB) * EXP(QNCHRT(3)/TCOMB)
         20 DENS = P/((10.73*1.8/454.) * TCCMB)
            TDROP = TRATE * DENS * A / GOLD
            TS = TCCMB + TDROP * (X-XCLD)
            RETURN
            END
```

```
                                                                                PAGE 0001
FORTRAN IV G LEVEL  19                 UPDATE
 0001             SUBROUTINE UPDATE(GO,YO,XZO,YNOO,TO,RATES,TB,G2,Y2,XZ2,YNO2,T2,
                 1                  NIND,NDEP,NCCMP,CPAVG,CPCOEF,IBOMB,SS,TI)
            C
            C
            C
            C
            C*******************************************************
            C*    THIS SUBROLTINE MIXES THE GAS STREAM AND THE      *
            C*    FUEL STREAM TC CCMPUTE A NEW TEMPERATURE AND      *
            C*    COMPOSITION.--IN THE TEMPERATURE CALCULATICN      *
            C*    THE HEAT OF VAPCRIZATICN/GASIFICATION IS TAKEN    *
            C*    INTO ACCOUNT.                                     *
            C*******************************************************
            C
            C
            C
 0002             DIMENSICN ICCDE( 6),YO( 2),XZO( 4),Y2(2),XZ2(4),CPCOEF(NCOMP,10),
                 1          CPAVG(NCOMP),XMOLE(6),YFUEL(2),XFUEL(4)
 0003             COMMON/AA/HVAP
 0004             COMMON/BB/TIME
            C     YO=MOLE FRACTICN OF INDEPENDENT CCMPONENT AT THE BEGGINING
            C        OF THE SLICE
            C     XZO=SIMILAR TO YO BUT FOR THE INDEPENDENT CCMPONENTS
            C     Y2=MOLE FRACTICN OF INC. CCMP. AT EXIT OF SLICE
            C     XZ2=MOLE FRACTICN CF DEP. CCMP. AT EXIT OF SLICE
            C
            C
            C
 0005         999 CONTINUE
 0006             NTOTAL=NIND + NDEP
            C
            C
 0007             YNOFL=0.
 0008             YFUEL(1)=0.
 0009             YFUEL(2)=0.
 0010             XFUEL(1)=1.0
 0011             XFUEL(2)=0.
 0012             XFUEL(3)=0.
 0013             XFUEL(4)=0.
            C
 0014             TR=298.
 0015             CALL MIX(GO,YO,XZO,YNCO,TO,RATES,YFUEL,XFUEL,YNOFL,TI,G2,Y2,XZ2,
                 1        YNC2,T2,NIND,NDEP,NCCMP,CPAVG,CPCOEF,IBOMB)
 0016             HEAT=RATES*HVAP
 0017             IF(SS .NE. 0.) GO TO 710
 0018             CALL CAVG(NCCMP,CPCOEF,CPAVG,TR,TB)
 0019             XCP4=CPAVG(4)
 0020             SNSBL=RATES*CPAVG(4)*(TB-TI)
 0021             TI=TB
 0022             HEAT=HEAT+SNSBL
 0023         710 CALL CAVG(NCOMP,CPCOEF,CPAVG,TR,T2)
 0024             CPMIX2=0.
 0025             DO 30 I=1,NTCTAL
 0026             IF(I.GT. NIND) GO TO 29
```

```
FORTRAN IV G LEVEL  19                  UPDATE                                   PAGE 0002
                 CPMIX2=CPMIX2+Y2(I)*CPAVG(I)
                 GO TO 30
              29 II=I-NIND
                 CPMIX2=CPMIX2+XZ2(II)*CPAVG(I)
              30 CONTINUE
                 DELT=HEAT/(G2*CPMIX2)
                 T2=T2-DELT
                 PRINT 90,T2,DELT
              90 FORMAT(//1X,'T2=',E14.6,'DELT=',E14.6/)
                 RETURN
                 END
```

```
 0001             SUBROUTINE SFRAY(AREA,STEP,RATES,NT,NSPRAY,TB,T,P,G)
            C
 0002             DIMENSICN AREAPO(10),EVAP(10),BURN(10),ERATE(10)
 0003             DIMENSION RF(10),RF2(10),RF3(10)
 0004             DIMENSION W(10)
 0005             DOUBLE PRECISICN EERATE
            C
            C**** THIS SUBROLTINE COMPUTES THE MOLES/SEC OF
            C     GAS GENERATED BY EITHER THE BURNING OF A
            C     LIQUID SPRAY GR A SCLID SPRAY
            C
 0006             COMMON/AB/R(10),RHCNV(10),NGROUP,NFNCTN,RHOP,AVGMW,
                 1          VP,      WDP(10),XNDP(10)
 0007             COMMON /EE/ FUEL
            C
            C     THE COMMCN BLCCK /AB/ IS LINKED TC SUBROUTINE ADATA
            C
 0008             REAL K
            C
            C        AVGMW=AVERAGE MCLECULAR WEIGHT OF GAS GIVEN OFF
            C        AREA=CROSS SECTICNAL AREA OF FLOW(FT**2)
            C        ERATE=EVAPCRATION RATE OF LIQUID SPRAY,OR
            C              GASIFICATICN RATE OF SOLIDS(MOLES/SEC). ERATE IS
            C        NSPRAY=1 (SPRAY IS LIQUID)
            C        NSPRAY=2 (SPRAY IS SCLID)
            C        NT=COUNTER
            C        R(I)=PARTICLE RADIUS (MICRONS)
            C        RHOP=PARTICLE DENSITY. ASSUMED TO BE
            C             UNIFCRMED FOR ALL PARTICLES(LBS/FT**3)
            C        VP=PARTICLE VELOCITY(FT/SEC)
            C        NGROUP=NO. CF DISCRETE PARTICLE SIZES GROUPS
            C               USED TO CHARACTERIZE THE DISTRIBUTION
            C               OF THE SPRAY. IT CANNOT EXCEED 10.
            C
 0009             PI=3.1416
 0010             XSQR4P=SQRT(4.*PI)
            C
            C        NFNCTN=0  VAPCRIZATICN/GASIFICATION RATE IS CONSTANT
            C        NFNCTN=1  VAPCRIZATION/GASIFICATION RATE IS NOT CONSTANT
            C        FUEL=TOTAL MOLES OF LIQUID/SOLID FUEL FED TO BOILER
            C        P=PRESSURE(PSI)
            C
            C**** INITIALIZATION
            C
            C
 0011             IF(NT.NE.0)GO TC 3
            C     FPI=4.*PI
 0012             FPI=12.5664
 0013             RR=1206.28
            C     RR=1206.28(CM**3-PSI/(GM-MOLE OK)
 0014             TFUEL=FUEL
 0015             SUMFUL=0.
            C
```

```
FORTRAN IV G LEVEL  19                SPRAY                                                    PAGE 0002
              C       WDP=WEIGHT DISTRIBUTICN OF PARTICLES
              C       XNOP=NUMBER DISTRIBUTICN OF PARTICLES/SEC
              C
 0016                 PI43RO=PI*4./3.*RHOP
 0017                 FAVGMW=FUEL*AVGMW
              C
              C******** CALCULATE THE PARTICLES/SEC OF FUEL XNDP(I) FOR
              C             EACH GRCUP OF PARTICLES BEING FED INTO THE BURNER.
              C             FORM THE CONTINUITY EQUATION WE KNOW THAT XDNP(I)
              C               IS CONSTANT.
              C
 0018                 DO 1 I=1,NGROUP
              C
              C------- CONVERT FROM MICRCNS TO FEET
              C
 0019                 RF(I)=R(I)/30.48E4
 0020                 RF2(I)=RF(I)*RF(I)
 0021                 RF3(I)=RF(I)*RF2(I)
 0022                 AREAPO(I)=FPI*RF2(I)
 0023               1 XNDP(I)=WDP(I)*FAVGMW/PI43RO/RF3(I)/454.
              C
              C       1 MICRON= 1./30.48E4 FEET
              C
              C       IF THE SPRAY IS A SOLID BYPASS LIQUID SPRAY CALCULATION.
              C
              C
              C
              C******** CALCULATE THE VELOCITY OF THE FUEL PARTICLES. IT
              C             IS ASSUMED THAT THESE PARTICLE MOVE AT THE VELO-
              C             CITY OF THE GAS STREAM ENTERING THE DIFFERENTIAL
              C             ELEMENT.
              C
 0024               3 VP=G*RR*T/P/28320./AREA
              C
              C
              C-------- SUBROUTINE VAPOR CALCULATES THE EVAPORATION
              C             RATE,EVAP, PER UNIT AREA OF LIQUID FOR EACH
              C           GROUP OF PARTICLES.
              C
 0025                 CALL VAPOR(RF,PI,VP,RHCP,STEP,NGRCUP,W)
              C
 0026                 WW=0.
 0027                 DO 27 I=1,NGRCUP
 0028                 WW=WW + W(I)*XNDP(I)
 0029              27 CONTINUE
 0030                 WW=WW*454./AVGMW
 0031                 RATES=WW
 0032                 EERATE=-WW
 0033                 SUMFUL=SUMFUL-EERATE
 0034                 IF(SUMFUL.GE.TFUEL)NSPRAY=0
 0035                 IF(SUMFUL.GT.TFUEL)RATES=RATES-(SUMFUL-TFUEL)
 0036                 DIVI=SUMFUL/TFUEL
 0037                 IF(DIVI.GE.0.9959)NSPRAY=0
```

```
                                                                                    PAGE 0003
FORTRAN IV G LEVEL  19                  SPRAY

 0038               NT=NT+1
 0039               IF(RATES.LT.1.)NSPRAY=0
 0040               PRINT 30
 0041            30 FORMAT(/2X,'PARTICLE RADIUS PARTICLE SURFACE EVAPORATION RATE DENS
                   1ITY FUNCTION PARTICLE VELOCITY  NO. OF GROUPS'/)
 0042               DO 50 I=1,NGROUP
 0043               R(I)=RF(I)*30.48E4
 0044               PRINT 31,R(I),VP,WW,NGROUP
 0045            31 FORMAT(1X,3E17.7,7X,I3)
 0046            50 CONTINUE
 0047               RETURN
 0048               END
```

```
FORTRAN IV G LEVEL  19                VAFOR                                              PAGE 0001

 0001                SUBROUTINE VAPOR(RF,PI,VP,RHOP,STEP,NGROUP,W)
             C
             C  THIS SUBROUTINE CALCULATES THE VAPORIZATION OF FUEL OIL DROPLETS
             C
 0002                COMMON /IJ/ VAPF
 0003                DIMENSION DELTA(10), D(10), DNEW(10), RF(10), W(10)
 0004                COMMON/BB/TIME
 0005                PRINT 50
 0006             50 FORMAT (2X, 'NGROUP', 5X, 'D', 10X, 'DNEW', 10X, 'DELTA', 10X,
                   1  'W', 12X, 'EVAP')
 0007            400 CONTINUE
 0008                X1=VAPF
 0009                DELT=STEP/VP
 0010                TIME=TIME + DELT
 0011                GROUP5=VAPF*TIME
 0012                DO 200 I = 1,NGROUP
 0013                D(I)=RF(I)*2.
             C
             C  CALCULATE NEW DIAMETER
             C
 0014                ARG =  D(I)**2 -  GROUP5
 0015                IF (ARG .LE. 0.0) ARG=1.E-40
 0016                DNEW(I) = SQRT(ARG)
             C
             C  CALCULATE CHANGES IN SURFACE
             C
 0017                DELTA(I)=PI*D(I)**2
             C
             C  CALCULATE TOTAL LBS EVAPORATED
             C
 0018                W(I) = RHCP * (PI/6) * (D(I)**3 - DNEW(I)**3)
             C
             C  CALCULATE VAPORIZATICN FLUX
             C
             C       EVAP(I)=W(I)/DELTA(I)/DELT
             C
             C  PRINT RESULTS
             C
 0019                RF(I)=DNEW(I)/2.
 0020                PRINT 100,I,D(I),DNEW(I),DELTA(I),W(I)
 0021            100 FORMAT ( 4X, I2, 5(1X, E12.5))
 0022            200 CONTINUE
 0023                RETURN
 0024                END
```

```
FORTRAN IV G LEVEL  19                  PCLUT                                            PAGE 0001

 0001              SUBROUTINE PCLUT(P,T,GOLD,G,YNOLD,STEP,A,YN2,YO2,YNO,YNOEQ,SS)
 0002              DOUBLE PRECISION ONE,TWO,FOUR,AAA,CCC,DELTAA,YYNO1,YYNO2,XXSQR
 0003              DOUBLE PRECISION VLUME,GG, AA4,AA2,YYO2,GGOLD,YYNOLD,AA3,AA1,
                  1                YYN2,XDSQ2,APRME,BPRME,CPRME,SSS
 0004              DOUBLE PRECISION GROUP1,GROUP3,GROUP4,GROUP5,DNODT,YYNO,YYO2EQ,
                  1                AA5,AA6,AA7,YYOH,YYH,GROUP6
 0005              COMMON/CD/YO2EQ
 0006              COMMON/EF/TEST1,KINJEC,KPASSS
 0007              COMMON/KDATA/TABLE(10,3),MODEL,NMAX1
             C
             C**** THIS SUBROUTINE COMPUTES THE MOLE FRACTION OF NITROGEN OXIDE ****
             C
             C     A=AREA OF FLOW(FT**2)
             C     G=MOLAR FLOW RATE OF GASES (MOLES/SEC)
             C     GOLD= MOLAR FLOW RATE OF GASES IN PREVIOUS SLICE
             C     YNO=MOLE FRACTION OF NO
             C     YNOEQ=EQUILIBRIUM MOLE FRACTION
             C     YNOLD=MOLE FRACTION OF NO IN PREVIOUS STEP
             C     YO2=MOLE FRACTION OF OXYGEN
             C     YN2=MOLE FRACTION OF NITROGEN
             C     P=PRESSURE(PSIA)
             C     T=TEMPERATURE(OK)
             C     STEP=INTEGRATION STEP SIZE(IN FEET)
             C     SS=DISTANCE FROM THE INLET(FEET)
             C     VLOCT=VELOCITY OF GAS(FT/SEC)
             C     YO2EQ=EQUILIBRIUM MOLE FRACTION OF OXYGEN
             C     XKO=EQUILIBRIUM OXYGEN DISSOCIATION CONSTANT
             C
 0008              IF(KPASSS.EQ.1)GO TO 1
 0009              IF(KINJEC.EQ.0.AND.YO2.LT.YO2EQ)YO2=YO2EQ
 0010            1 RR=1206.28
             C
             C     RR=1206.28(CM**3-PSI/(OK-GM-MOLE))
 0011              R=1.987
             C     R=1.987(CALORIES/(GM-MOLE-OK))
 0012              PRT=P/(RR*T)
 0013              PRT25=PRT**2.500
             C
             C**** COMPUTE THE MOLE FRACTION OF NO
             C
             C     GOLD*YNOLD - G*YNO +A*STEP*RATE OF NO = 0
             C     THE ABOVE EXPRESSION IS THE DIFFERENTIAL
             C     MASS BALANCE ON NO
             C
 0014              XKO=25.*EXP(-118600./(R*T))
             C
             C
 0015              RT=R*T
             C
             C-------- LEEDS DATA
             C
 0016              XK3=1.36E14*EXP(-75400./(R*T))
 0017              XK4=3.1E13*EXP(-334./(R*T))
 0018              XK5=6.43E9*T*EXP(-6250./(R*T))
 0019              XK6=1.55E9*T*EXP(-38640./(R*T))
 0020              A1=2.*SQRT(XKO)*XK3*XK5*PRT25
 0021              A2=2.*SQRT(XKO)*XK4*XK6*PRT25
 0022              A3=XK5*PRT
 0023              A4=XK4*PRT
 0024              AA1=A1
 0025              AA2=A2
 0026              AA3=A3
 0027              AA4=A4
            C
            C         THE ABOVE CCNSTANTS WERE TAKEN FROM THE THIRD
            C         MONTHLY REPORT TO NAPCA---'SYSTEMS STUCY OF
            C         NITROGEN CXIDE CCNTROL METHODS FOR STATIONARY
            C         SOURCES--'PHASE II----CONTRACT CPA 70-90,9/10/70.
            C
 0028              VOLUME=A*STEP*28320.
 0029              VLUME=VOLUME
            C
            C         THE FACTOR 28320. IS TO CONVERT FROM CM**3 TO FT**3.
            C
 0030              GG=G
 0031              YYO2=YO2
.0032              GGOLD=GOLD
 0033              YYNOLD=YNOLD
 0034              YYN2=YN2
 0035              XDSO2=DSQRT(YYO2)
 0036              GROUP1=AA1*YYN2*YYC2*XDSO2
 0037              GROUP3=AA3*YYO2
 0038              APRME=-(GG*AA4 + VLUME*AA2*XDSO2)
 0039              BPRME=GGOLD*YYNCLD*AA4-GG*GROUP3
 0040              CPRME=GGOLD*YYNOLD*GROUP3 + VLUME*GROUP1
            C
            C      WHEN MODEL=2 THE GH REACTICN IS INCLUDED
 0041              IF(MODEL.NE.2)GO TO 10
 0042              A5=2.*SQRT(XKO)*XK3*XK7*PRT25
 0043              PRT3=PRT*PRT*PRT
 0044              A6=XK4*XK8*PRT3
 0045              A7=XK7*PRT
 0046              AA5=A5
 0047              AA6=A6
 0048              AA7=A7
            C
            C      INTERPOLATE FCR MOLE FRACTION OF OH AND H.
            C
            C
            C      TABLE(KPOINT,1)=TEMPERATURE VECTOR
            C      TABLE(KPOINT,2)=OH CCNCENTRATION VECTOR
            C      TABLE(KPOINT,3)=H CONCENTRATION VECTOR
 0049              CALL INTRPL(T,TABLE(1,1),TABLE(1,2),NMAX1,YOH)
 0050              YYOH=YOH
 0051              CALL INTRPL(T,TABLE(1,1),TABLE(1,3),NMAX1,YH)
 0052              YYH=YH
```

```
FORTRAN IV G LEVEL  19                PCLUT
                                                                    PAGE 0003
          C      USE SUBROUTINE INTERPCLATE
          C      YYOH=YOH  AND YYH=YH
                 GROUP4=VLUME*AA6*YYH
                 GROUP5=   AA7*YYOH
                 GROUP6=VLUME*AA5*YYN2*YYOH*XDSO2
                 APRME=APRME + GROUP4
                 BPRME=BPRME -GG*GROUP5
                 CPRME=CPRME +GRCUP6 +GGOLD*YYNOLD*GROUP5
              10 AAA=APRME/BPRME
                 CCC=CPRME/BPRME
                 VLOCT=G/PRT/28320./A
                 ONE=1.0000000
                 TWO=2.000000C
                 FOUR=4.000C000
                 DELTAA=FCUR*AAA*CCC
                 XXSQR=DSQRT(CNE-DELTAA)
                 YYNO1=(-CNE+XXSQR)/(TWG*AAA)
                 YYNO2=(-CNE-XXSQR)/(THC*AAA)
          C
          C---------FIND VALID RCOT
          C
                 IF(YYNO1.GE.C..AND.YYNO1.LT.1.)YYNO=YYNO1
                 IF(YYNO2.GE.O..AND.YYNO2.LT.1.)YYNC=YYNO2
                 YNO=YYNO
          C
          C
          C---------CORRECT OXYGEN CCNCENTRATICN BY SUBTRACTING AMOUNT
          C         CONSUMED BY THE NITROGEN OXYGEN REACTION.
          C
          C
          C         DNODT=GENERATICN RATE OF NITROGEN OXIDE(GM-MOLES/CM**3-SEC)
          C
               2 YNOEQ= 4.68*EXP(-21700./(R*T))*(YN2**0.5)*(YO2**0.5)
                 IF(SS.EQ.0.)TIME=0.
                 DLTIME=STEP/VLCCT
                 TIME=TIME+DLTIME
                 IF(SS.LT.TEST1)RETURN
                 DNODT=(GROUP1-AA2*YYNO**2*XDSO2)/(GROUP3+AA4*YYNO)
                 IF(KPASSS.EQ.0)GO TO 3
                 IF(KINJEC.EQ.1)YO2EQ=YC2
                 IF(KINJEC.EQ.1)YYO2EQ=YO2EQ
                 IF(KINJEC.EQ.1)KINJEC=0
                 YYO2EQ=YYO2EQ-DNODT*VLUME/GG/2.
                 YO2EQ=YYO2EQ
                 YO2=YO2EQ
                 RETURN
               3 CONTINUE
                 IF(YO2EQ.EQ.C.)YO2EQ=YC2
                 YYO2=YO2EQ
                 YYO2=YYO2-DNODT*VLUME/GG/2.
                 IF(YYO2.LT.0.)YYO2=0.
                 YO2EQ=YYO2
                 YO2=YYO2
```

```
                                                                                  PAGE 0004
FORTRAN IV G LEVEL  19                  PCLUT

 0093            RETURN
 0094            END
```

D.3 Sample Output

```
  COMBUSTION/POLLUTION MODEL--- MGM-6 0.5*FL(105),FR(.95),RL(.10),RR(.10),  LEEDS DATA

          DECK 3347

        INPUT SUMMARY
   ***************************

CARD 1 - OPTIONS
----------------

        0 WALL TEMPERATURE PROFILE NOT SPECIFIED
        2 GAS TEMPERATURE PROFILE COMPUTED FROM QR
        0 HEAT FLUX PROFILE NOT SPECIFIED
        0 NO. OF SECONDARY INJECTION PTS.

CARD 2 - STOICHIOMETRIC COEFFICIENTS (FUEL COMBUSTION)
------------------------------------------------------

      1.000 FUEL COEFFICIENT
      1.500 O2 COEFFICIENT
      1.000 CO COEFFICIENT
      2.000 H2O COEFFICIENT

CARD 3 - PHYSICAL CONDITIONS OF INLET GAS MIXTURE
-------------------------------------------------
                  ** FUEL LEAN **
                     ---------

   5498.012 FLOW RATE (G-MOLES/SEC)
    533.000 TEMPERATURE (K)
     14.700 PRESSURE(PSIA)
      0.0   ADIABATIC FLAME TEMPERATURE AT INLET (K)

                  ** FUEL RICH **
                     ---------

   5021.564 FLOW RATE (G-MOLES/SEC)
    533.000 TEMPERATURE (K)
     14.700 PRESSURE(PSIA)
      0.0   ADIABATIC FLAME TEMPERATURE AT INLET (K)

CARD 4 - INLET GAS COMPOSITION
------------------------------

                  ** FUEL LEAN **
                     ---------

      0.191 MOLE FRACTION OF O2
      0.0   MOLE FRACTION OF CO2
      0.091 MOLE FRACTION OF FUEL
      0.0   MOLE FRACTION OF CO
      0.0   MOLE FRACTION OF H2O
      0.718 MOLE FRACTION OF N2
      0.0   MOLE FRACTION OF NO

                  ** FUEL RICH **
                     ---------

      0.189 MOLE FRACTION OF O2
      0.0   MOLE FRACTION OF CO2
      0.100 MOLE FRACTION OF FUEL
      0.0   MOLE FRACTION OF CO
      0.0   MOLE FRACTION OF H2O
      0.711 MOLE FRACTION OF N2
      0.0   MOLE FRACTION OF NO

CARD 7 - KINETIC RATE CONSTANTS FOR FUEL COMBUSTION
---------------------------------------------------

    0.47E 16 FREQUENCY FACTOR
   56600.000 ACTIVATION ENERGY
       0.500 O2 EXPONENT
       1.000 FUEL EXPONENT
       0.500 H2O EXPONENT

CARD 8 - KINETIC RATE CONSTANTS FOR CO COMBUSTION
-------------------------------------------------

    0.18E 11 FREQUENCY FACTOR
   25000.000 ACTIVATION ENERGY
       0.500 O2 EXPONENT
       1.000 CO EXPONENT
       0.500 H2O EXPONENT

CARD 9.5 - QUENCH RATE CONSTANTS
--------------------------------

   -1893.000 FIRST COEFFICIENT
       2.622 SECOND COEFFICIENT
      -0.001 THIRD COEFFICIENT

  QUADRATIC RATE TO BE USED

CARD 10 - COMBUSTOR PROFILES
----------------------------

    DISTANCE   CROSS-SECTIONAL AREA   PERIMETER   WALL TEMPERATURE   GAS TEMPERATURE      HEAT FLUX
     (FEET)           (FT2)             (FEET)          (K)               (K)          (KCAL/FT2-SEC)
     ------           ----              ------          ---               ---          --------------

       0.0          1320.000           145.200          0.0               0.0               0.0
      50.000        1320.000           145.200          0.0               0.0               0.0

CARD 11 - COMBUSTOR LENGTH AND PRINOUT INTERVAL
-----------------------------------------------

       40.020 REACTOR LENGTH (FEET)
        0.200 PRINTOUT INTERVAL (FEET)
        0.020INTEGRATION INTERVAL (FEET)

CARD 12 - HEAT OF REACTION AT 298K
----------------------------------

    -124.118 HEAT OF REACTION FOR FUEL COMBUSTION
     -67.636 HEAT OF REACTION FOR CO COMBUSTION

CARD 13 - HEAT CAPACITY DATA FOR FUEL (298K TO 1200K)
-----------------------------------------------------

         11 NO. OF HEAT CAPACITY DATA POINTS FOR FUEL (298K TO 1200K)
```

```
CARD 14 - HEAT CAPACITY DATA POINTS FOR FUEL (298K TO 1200K)
------------------------------------------------------------

  TEMPERATURE (K)    HEAT CAPACITY OF FUEL (CAL/G-MOLES, K)
  ---------------    --------------------------------------

      298.000                     8.518
      300.000                     8.538
      400.000                     9.680
      500.000                    11.076
      600.000                    12.483
      700.000                    13.813
      800.000                    15.041
      900.000                    16.157
     1000.000                    17.160
     1100.000                    18.052
     1200.000                    18.842

CARD 15 - HEAT CAPACITY DATA FOR FUEL (T > 1200K)
-------------------------------------------------

        18 NO. OF HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200K)

CARD 16 - HEAT CAPACITY DATA POINTS FOR FUEL (T > 1200K)
--------------------------------------------------------

  TEMPERATURE (K)    HEAT CAPACITY OF FUEL (CAL/G-MOLES,K)
  ---------------    -------------------------------------

     1300.000                    19.538
     1400.000                    20.150
     1500.000                    20.688
     1600.000                    21.161
     1700.000                    21.579
     1800.000                    21.947
     1900.000                    22.273
     2000.000                    22.562
     2100.000                    22.820
     2200.000                    23.050
     2300.000                    23.256
     2400.000                    23.441
     2500.000                    23.608
     2600.000                    23.758
     2700.000                    23.894
     2800.000                    24.018
     2900.000                    24.131
     3000.000                    24.233


        FRACTION OF FUEL LEAN STREAM TRANSFERRED TO THE RICH ZONE = 0.1000E 00
        FRACTION OF FUEL RICH STREAM TRANSFERRED TO THE LEAN ZONE = 0.1000E 00
        FRACTION OF VOLUME IN FUEL LEAN ZONE = 0.5000E 00
```

```
                                          COMBUSTION/POLLUTION MODEL
                                               CUTPUT SUMMARY
                                          ****************************

               ADIABATIC FLAME TEMPERATURE FOR INLET GAS MIXTURE =    2416.87 K

DISTANCE     FLOW RATE         T           G2           CO2          FUEL          CO          H2O          N2           NO          NO(EQ)
  (FT)     (G-MOLS/SEC)       (K)        ----------------------------------------------(MOLE FRACTION)-------------------------------------------

      COMPOSITION OF FUEL LEAN STREAM

0.0             5498.        533.0      0.19C9       0.0          0.9089E-01  0.0          0.0          0.7182       0.0          0.0

      COMPOSITICN OF FUEL RICH STREAM

0.0             5022.        533.C      0.1891       0.0          0.9950E-01  0.0          0.0          0.7114       C.0          0.0

      COMPOSITION OF FUEL LEAN STREAP

0.2000E-01    5485.         2327.       0.1310E-01  0.8001E-01  0.4418E-04  0.1102E-01  0.1821       0.7137       0.1799E-04  0.4144E-02

      COMPOSITICN OF FUEL RICH STREAP

0.2000E-01    5117.         2405.       0.2411E-C2  0.7735E-01  0.7363E-04  0.2020E-01  0.1951       0.7048       0.1917E-04  0.2060E-02

      COMPOSITION OF FUEL LEAN STREAP

0.4000E-01    5424.         2333.       0.7229E-02  0.9021E-01  0.2774E-07  0.1846E-C2  0.1841       0.7166       0.3239E-04  0.3121E-02

      COMPOSITION OF FUEL RICH STREAM

0.4000E-01    5137.         2396.       0.4050E-04  0.8464E-01  0.4293E-06  0.1263E-01  0.1946       0.7081       0.1965E-04  0.2637E-03

      COMPOSITIGN OF FUEL LEAN STREAP
```

```
 0.6000E-01   5392.       2337.      0.5459E-02  0.9212E-01  0.2002E-10  0.5969E-03  0.1852      0.7166      0.4411E-04  0.2738E-02

     COMPOSITION OF FUEL RICH STREAM

 0.6000E-01   5155.       2389.      0.2923E-05  0.8669E-01  0.9676E-08  0.1017E-01  0.1937      0.7094      0.2089E-04  0.6980E-04

FUEL IS EXHAUSTED--PROCEED TO MIX WITH NO COMBUSTION REACTIONS


     COMPOSITION OF FUEL LEAN STREAM

 0.8000E-01   5370.       2341.      0.4976E-02  0.9165E-01  0.8627E-09  0.1432E-02  0.1859      0.7159      0.5464E-04  0.2633E-02

     COMPOSITION OF FUEL RICH STREAM

 0.8000E-01   5177.       2383.      0.5168E-03  0.8720E-01  0.8762E-08  0.9262E-02  0.1929      0.7101      0.2839E-04  0.9199E-03

     COMPOSITION OF FUEL LEAN STREAM

 0.2200       5297.       2354.      0.3295E-02  0.9001E-01  0.3775E-08  0.4319E-02  0.1885      0.7138      0.1191E-03  0.2194E-02

     COMPOSITION OF FUEL RICH STREAM

 0.2200       5250.       2364.      0.2205E-02  0.8892E-01  0.5714E-08  0.6240E-02  0.1902      0.7123      0.1034E-03  0.1830E-02

     COMPOSITION OF FUEL LEAN STREAM

 0.4200       5277.       2354.      0.2782E-02  0.8954E-01  0.4610E-08  0.5146E-02  0.1892      0.7131      0.1985E-03  0.2016E-02

     COMPOSITION OF FUEL RICH STREAM

 0.4200       5270.       2355.      0.2636E-02  0.8939E-01  0.4872E-08  0.5406E-02  0.1895      0.7129      0.1947E-03  0.1968E-02

        FUEL RICH AND FUEL LEAN STREAM HAVE MERGED
```

```
0.6000   0.1055E 05  2351.   0.2678E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7130   0.2598E-03  0.1970E-02
0.6200   0.1055E 05  2351.   0.2674E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7130   0.2670E-03  0.1964E-02
0.8200   0.1055E 05  2346.   0.2642E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7129   0.3319E-03  0.1934E-02
 1.020   0.1055E 05  2341.   0.2614E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7129   0.3869E-03  0.1907E-02
 1.220   0.1055E 05  2337.   0.2590E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7129   0.4344E-03  0.1881E-02
 1.420   0.1055E 05  2332.   0.2570E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7129   0.4759E-03  0.1856E-02
 1.620   0.1055E 05  2328.   0.2551E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.5125E-03  0.1833E-02
 1.820   0.1055E 05  2323.   0.2535E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.5451E-03  0.1810E-02
 2.020   0.1055E 05  2319.   0.2520E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.5742E-03  0.1789E-02
 2.220   0.1055E 05  2314.   0.2507E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.6004E-03  0.1768E-02
 2.420   0.1055E 05  2310.   0.2495E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.6240E-03  0.1748E-02
 2.620   0.1055E 05  2306.   0.2485E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.6454E-03  0.1729E-02
 2.820   0.1055E 05  2301.   0.2475E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7128   0.6649E-03  0.1710E-02
 3.020   0.1055E 05  2297.   0.2466E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.6826E-03  0.1691E-02
 3.220   0.1055E 05  2293.   0.2458E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.6988E-03  0.1674E-02
 3.420   0.1055E 05  2288.   0.2451E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7137E-03  0.1656E-02
 3.620   0.1055E 05  2284.   0.2444E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7272E-03  0.1639E-02
 3.820   0.1055E 05  2280.   0.2438E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7397E-03  0.1623E-02
 4.020   0.1055E 05  2276.   0.2432E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7512E-03  0.1606E-02
 4.220   0.1055E 05  2271.   0.2427E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7618E-03  0.1590E-02
 4.420   0.1055E 05  2267.   0.2422E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7715E-03  0.1575E-02
 4.620   0.1055E 05  2263.   0.2417E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7805E-03  0.1560E-02
 4.820   0.1055E 05  2259.   0.2413E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7888E-03  0.1545E-02
 5.020   0.1055E 05  2255.   0.2409E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.7965E-03  0.1530E-02
 5.220   0.1055E 05  2251.   0.2406E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8036E-03  0.1515E-02
 5.420   0.1055E 05  2247.   0.2402E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8101E-03  0.1501E-02
 5.620   0.1055E 05  2243.   0.2399E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8162E-03  0.1487E-02
 5.820   0.1055E 05  2239.   0.2396E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8219E-03  0.1473E-02
 6.020   0.1055E 05  2235.   0.2394E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8271E-03  0.1460E-02
 6.220   0.1055E 05   2231.   0.2391E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8320E-03  0.1446E-02
 6.420   0.1055E 05   2227.   0.2389E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8365E-03  0.1433E-02
 6.620   0.1055E 05   2223.   0.2387E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8406E-03  0.1420E-02
 6.820   0.1055E 05   2219.   0.2385E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8445E-03  0.1407E-02
 7.020   0.1055E 05   2215.   0.2383E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8481E-03  0.1395E-02
 7.220   0.1055E 05   2211.   0.2382E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8515E-03  0.1382E-02
 7.420   0.1055E 05   2207.   0.2380E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8546E-03  0.1370E-02
 7.620   0.1055E 05   2204.   0.2379E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8575E-03  0.1358E-02
 7.820   0.1055E 05   2200.   0.2377E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8602E-03  0.1346E-02
 8.020   0.1055E 05   2196.   0.2376E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7127   0.8627E-03  0.1334E-02
 8.220   0.1055E 05   2192.   0.2375E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8650E-03  0.1322E-02
 8.420   0.1055E 05   2188.   0.2374E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8672E-03  0.1311E-02
 8.620   0.1055E 05   2185.   0.2373E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8692E-03  0.1299E-02
 8.820   0.1055E 05   2181.   0.2372E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8710E-03  0.1288E-02
 9.020   0.1055E 05   2177.   0.2371E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8728E-03  0.1277E-02
 9.220   0.1055E 05   2174.   0.2370E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8744E-03  0.1266E-02
 9.420   0.1055E 05   2170.   0.2369E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8759E-03  0.1255E-02
 9.620   0.1055E 05   2166.   0.2369E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8772E-03  0.1245E-02
 9.820   0.1055E 05   2163.   0.2368E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8785E-03  0.1234E-02
10.02    0.1055E 05   2159.   0.2368E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8797E-03  0.1223E-02
10.22    0.1055E 05   2156.   0.2367E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8808E-03  0.1213E-02
10.42    0.1055E 05   2152.   0.2366E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8818E-03  0.1203E-02
10.62    0.1055E 05   2149.   0.2366E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8828E-03  0.1193E-02
10.82    0.1055E 05   2145.   0.2366E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8837E-03  0.1183E-02
11.02    0.1055E 05   2142.   0.2365E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8845E-03  0.1173E-02
11.22    0.1055E 05   2138.   0.2365E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8852E-03  0.1163E-02
11.42    0.1055E 05   2135.   0.2364E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8859E-03  0.1153E-02
11.62    0.1055E 05   2131.   0.2364E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8866E-03  0.1144E-02
11.82    0.1055E 05   2128.   0.2364E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8872E-03  0.1134E-02
12.02    0.1055E 05   2124.   0.2364E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8877E-03  0.1125E-02
12.22    0.1055E 05   2121.   0.2363E-02  0.8946E-01  0.4741E-08  0.5276E-02  0.1894   0.7126   0.8882E-03  0.1116E-02
```

APPENDIX E

ILLUSTRATIVE PHOTOGRAPHS OF LABORATORY COMBUSTION EQUIPMENT

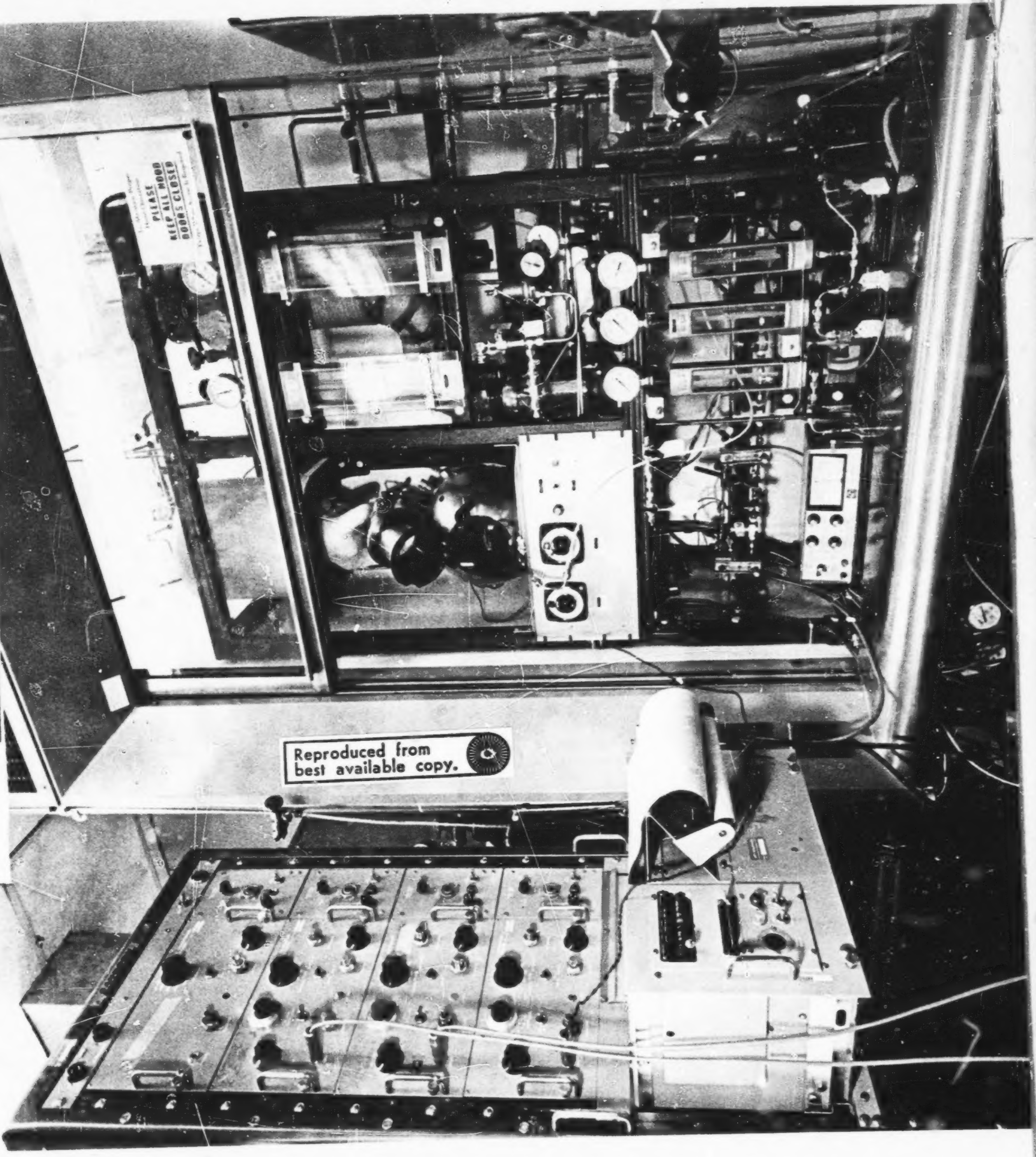
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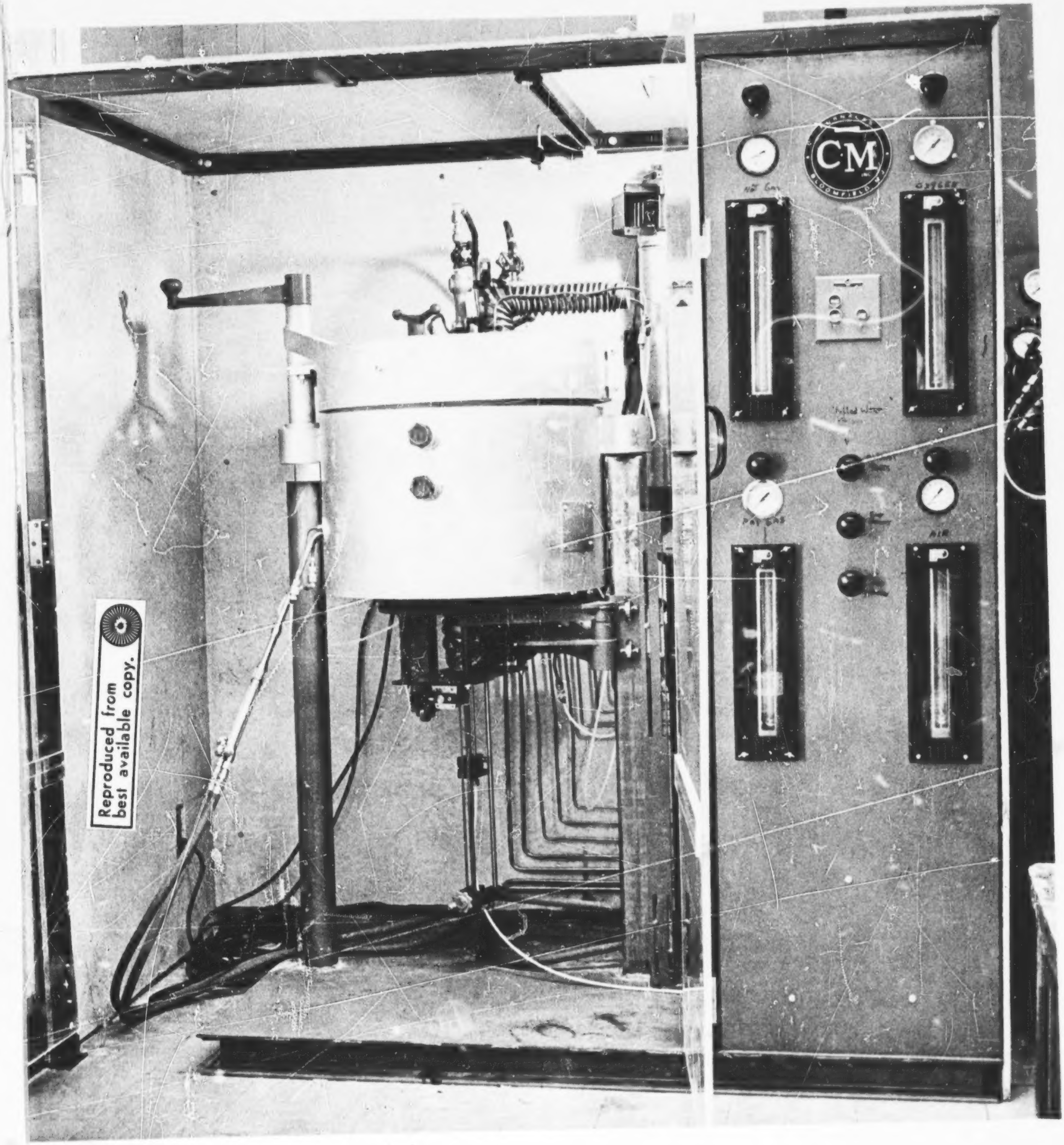
FIGURE E-1

THE JET STIRRED COMBUSTOR

FIGURE E-2

THE MULTIBURNER


CM
BLOOMFIELD N.J.
Nat Gas
OXYGEN
Chilled Water
AIR

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13. ABSTRACT

This report summarizes the findings in the laboratory studies and mathematical modeling portions of Phase II of a "Systems Study of Nitrogen Oxide Control Methods for Stationary Sources" (Contract CPA 70-90). Laboratory studies were conducted to investigate the basic factors affecting nitrogen oxide formation in the combustion of fossil fuels. A jet-stirred combustor and a multiburner (so-named because of its ability to burn gas, oil or pulverized coal fuels) were used in these studies. The first-generation model of NO_x formation and decomposition in combustion processes was extended.

The jet stirred combustor was used to study NO_x emissions from combustion under kinetically limited conditions. The key findings of these studies with the jet-stirred combustor are as follows:

- At the very short residence times prevailing in the jet-stirred combustor (on the order of 2 msec), substantial quantities of NO_x are formed with methane as the fuel, under stoichiometric and excess air firing conditions. (In fact, peak NO_x concentrations have been measured under slightly fuel rich conditions. The NO_x concentrations measured exceed those based on the Zeldovich mechanism in many cases by more than an order of magnitude, indicating that coupling occurs between NO_x formation and combustion kinetics.

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ABSTRACT (Continued)

- With carbon monoxide as the fuel, the NO_x emissions from the jet-stirred combustor are very similar to those obtained with methane fuel, at equivalent mixture ratios and slightly higher temperatures.

- With hydrogen as the fuel, the NO_x emissions are reduced to much lower levels at all mixture ratios compared with methane at the same temperatures. Good circumstantial evidence for the coupling between NO_x and combustion kinetics has been obtained in experiments in which methane or carbon monoxide was mixed with the hydrogen fuel. In the presence of small amounts of these gases, the NO_x concentrations measured increased when compared to the results for hydrogen at the same mixture ratio.

- Under fuel rich conditions, the amount of NO_x drops off precipitiously in the jet-stirred combustor. This finding provides support for the optimized design of the two-stage combustion technique for NO_x emission control from combustion sources.

- All of the "bond-type" additives (NO, NO_2, NH_3 and $(CN)_2$ and CH_3NH_2) result in nearly equivalent NO_x emissions, operating the jet-stirred combustor with excess air. The conversion between additive input and NO_x output is constant as the additive level is increased up to 3000 ppm equivalent NO_x. (Slight falloff was noted for $(CN)_2$ above 3000 ppm.)

- The fraction of N-bond additives oxidized to NO_x is sharply decreased on the fuel-rich side. This finding is of practical significance, because of the potential of fuel-rich combustion followed by second-stage air injection to control NO_x emissions from both atmospheric N_2-fixation and fuel nitrogen oxidation.

Preliminary experiments were performed with the multiburner which indicated the influence of heat losses and residence time on NO_x emissions in combustion of methane/air. The multiburner has also been used as a rudimentary flow reactor for the formation of nitrogen oxides in air at high temperatures.

The mathematical model has been extended to allow calculations of NO formation under fuel-rich conditions. Particle combustion capability has been incorporated into the model and mixing effects can be handled with the macro-mixing option. This latter feature allows consideration of such combustion modifications as off-stoichiometric combustion. Test cases have been run for the above options which indicate the correct order of magnitude predictions and the correct directional effect of modifications.